

Supporting Information

Electrochromism of Alkylene-Linked Discrete Chromophore Polymers with Broad Radical Cation Absorptions

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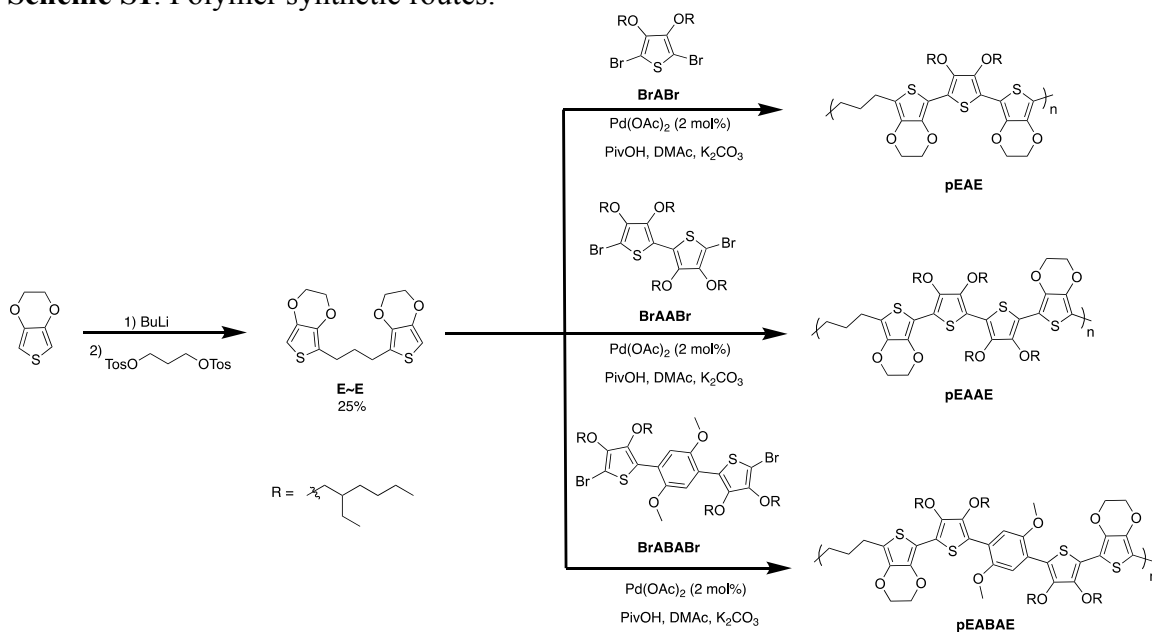
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30597

Monomer Synthesis and Primary Characterization

All reagents and starting materials were purchased from commercial sources and used without further purification, unless otherwise noted. 2,5-dibromo-3,4-bis(2-ethylhexyloxy)thiophene (**BrABr**), 2,5'-dibromo-3,3',4,4'-tetrakis((2-ethylhexyl)oxy)-2,2'-bithiophene (**BrAABr**), and **BrABABr** were used as produced from previous literature procedures.¹⁻³ All reactions carried out under an argon atmosphere unless otherwise mentioned.

Scheme S1. Polymer synthetic routes.



E~E. Into a flame dried 50 mL schlenk flask with a magnetic stir bar was added freshly distilled 3,4-ethylenedioxythiophene (5.007 g, 35.17 mmol) and 30 mL of dry THF. The flask was purged with Ar and the mixture was cooled to -78°C in a dry ice-acetone bath. To the flask was added nBuLi (2.5 M, 14.06 mL, 35.15 mmol) drop wise over 1 hour. The solution stirred for 1 additional hour at -78°C and 1,3-propyleneditosylate (6.59 g, 17.16 mmol) was added all at once. The solution was allowed to warm to room temperature as it stirred for 12 hours. The reaction mixture was slowly quenched with 100 mL of DI water and extracted with diethyl ether (3 x 100 mL). The organic fractions were washed with water (2x 100), dried over MgSO₄, and solvent removed under reduced pressure. The compound was purified via fractional vacuum distillation using a kugelrohr (bp ~150°C at 10 mbar) to give a clear oil. ¹H-NMR (CDCl₃, ppm): δ 6.12 (s, 2H), 4.17 (s, 8H), 2.72-2.27 (t, 4H, J=1.5 Hz), 1.97-1.86 (q, 2H, J=1.5 Hz); ¹³C-NMR (CDCl₃, ppm): δ 141.5, 137.6, 117.5, 95.3, 65.0, 65.5, 31.0, 25.5. HRMS: Calculated Mass = 324.0489 Da, Measured Mass = 324.0490 Da.

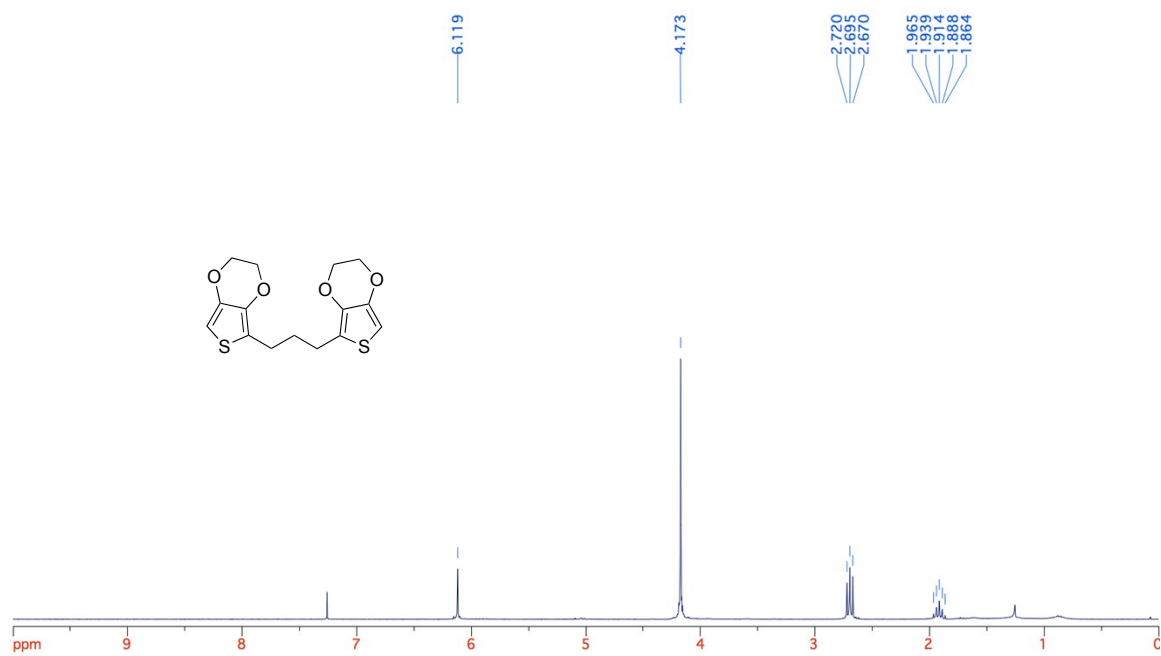


Figure S1. ¹H NMR of **E~E**

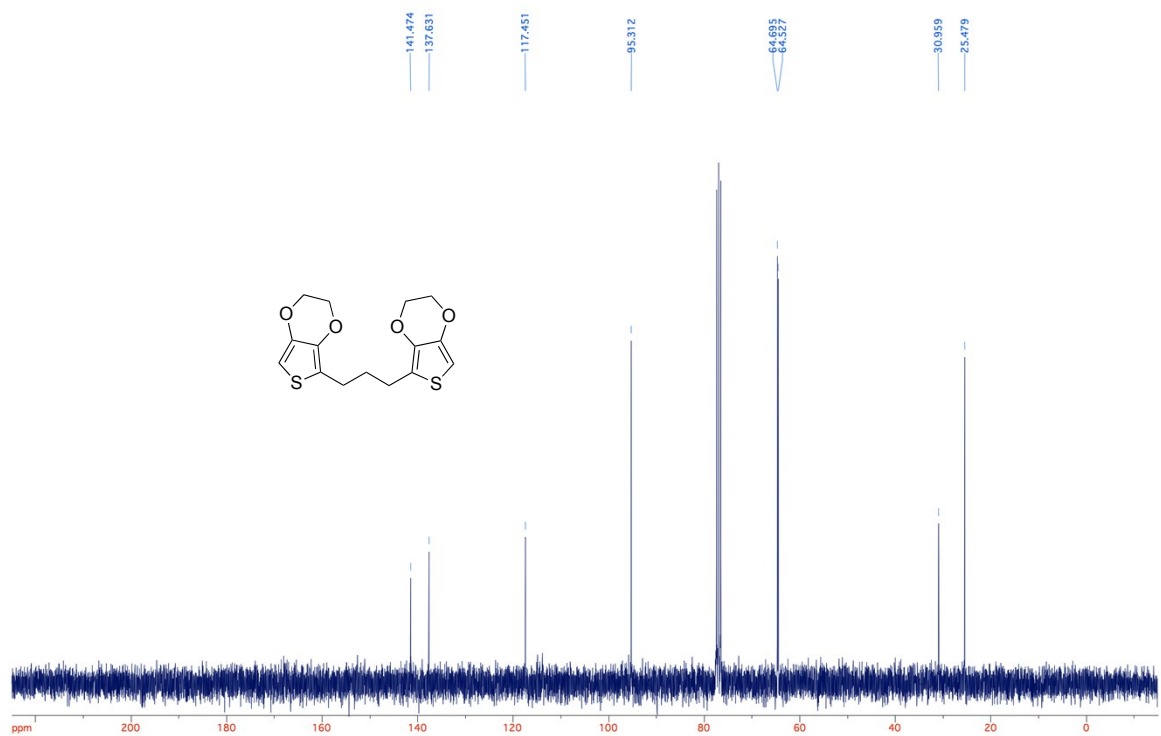


Figure S2. ¹³C NMR of **E~E**

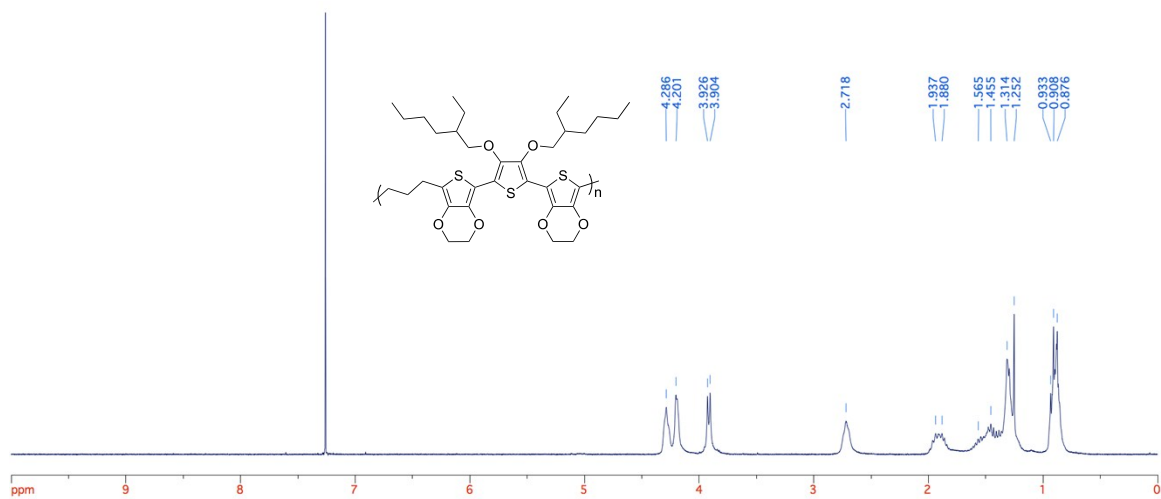


Figure S3. ^1H NMR of **pEAE**

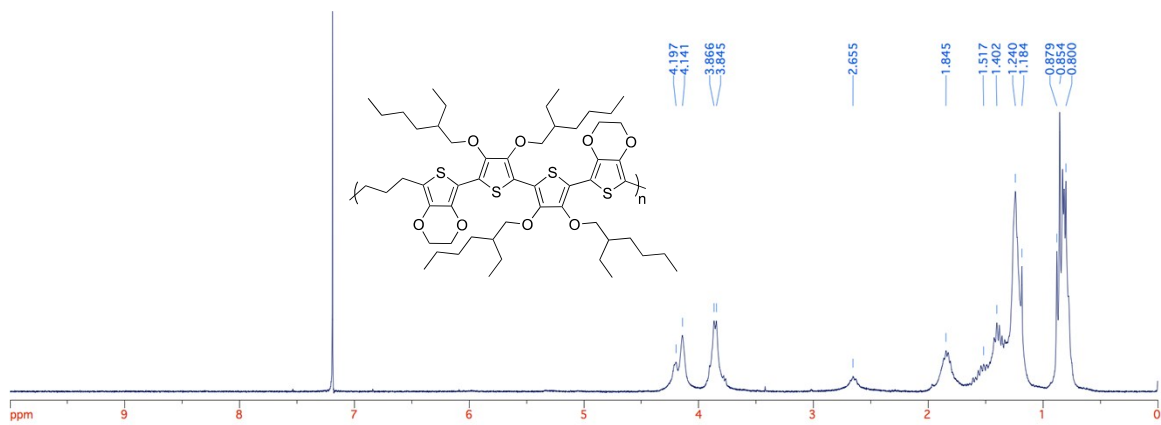


Figure S4. ^1H NMR of **pEAAE**

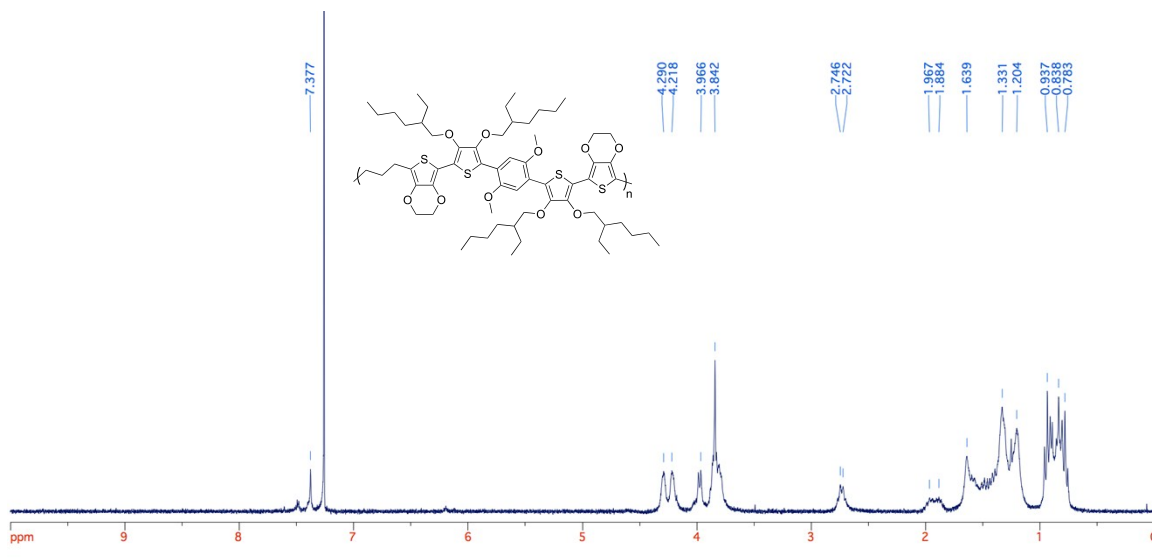


Figure S5. ^1H NMR of pEABAE

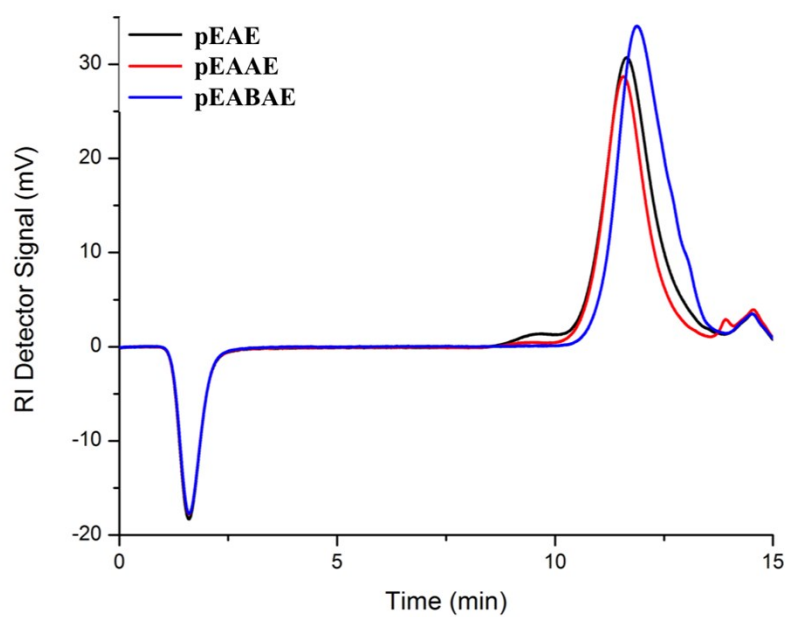


Figure S6. Gel permeation chromatography (GPC) results of the family of polymers in CHCl_3 at 40°C

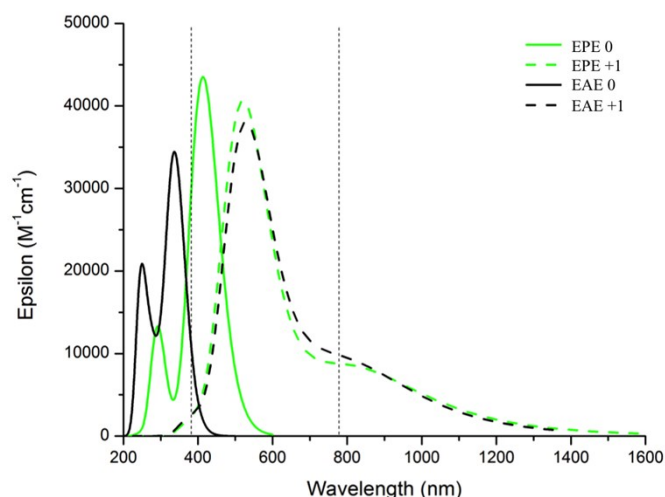


Figure S7. UV-Vis-NIR calculated spectra of **EPE** and **EAE** in the neutral (solid) and radical cation (dashed) states. Vertical dotted lines indicate the visible range of 380-780 nm

Quantum Chemical Calculations Supplemental

The functional and basis set mPW1PBE/cc-PVDZ include the following details. With respect to mPW1PBE, this *one*-parameter, hybrid functional is a variation of the *Perdew-Wang* exchange with *PBE* correlation.⁴ The basis set, cc-PVDZ, is a correlation consistent (cc), *double-zeta* basis set which includes valence *polarization* functions (PV) for specific atoms.⁵

I. Optimized Coordinates:

Keywords/settings: opt freq cc-pvdz scrf=(cpcm,solvent=dichloromethane)
geom=connectivity mpw1pbe

a. EPE

i. Neutral

C	-0.96890300	1.64386100	-0.81289500
C	-0.54561000	0.37691900	-0.45753900
S	0.00001200	2.85494300	0.00000400
C	0.54561100	0.37691400	0.45754800
O	-1.16663800	-0.73288200	-0.93120000
C	0.96891500	1.64385200	0.81290300
O	1.16663000	-0.73289200	0.93120800
C	-0.32353200	-1.84866700	-1.21961500
C	0.32351500	-1.84867200	1.21962000
H	-0.86653700	-2.43959100	-1.96972700
H	0.61415000	-1.49208200	-1.67005000
C	-0.00001100	-2.72263700	0.00000100
H	0.86651400	-2.43960100	1.96973200
H	-0.61416600	-1.49208100	1.67005400
C	-1.16244100	-3.64688800	0.37987200
C	1.16241500	-3.64689300	-0.37987200
H	-1.36897400	-4.33857700	-0.46099600

H	-0.86362500	-4.27457100	1.24454100
O	-2.30953700	-2.90345100	0.69542200
H	1.36894500	-4.33858400	0.46099400
H	0.86359500	-4.27457300	-1.24454200
O	2.30951400	-2.90346000	-0.69542200
C	-3.38242900	-3.72363300	1.11161600
C	3.38240100	-3.72364600	-1.11162000
H	-3.62787000	-4.45481200	0.31573500
H	-3.08229500	-4.30977600	2.00254000
H	3.62784100	-4.45482800	-0.31574200
H	3.08226300	-4.30978600	-2.00254400
C	4.59050300	-2.85985100	-1.44611400
C	5.69845400	-3.74266600	-2.03054800
C	6.92231900	-2.98659900	-2.53535300
H	6.01535000	-4.49056800	-1.28196500
H	5.27397800	-4.32406300	-2.86803500
C	7.94650500	-3.88951100	-3.21457700
H	6.60036300	-2.20253400	-3.24447000
H	7.41169700	-2.45661400	-1.70026700
H	8.25884700	-4.67842000	-2.50792000
H	7.46464800	-4.41466500	-4.05791500
C	-4.59052800	-2.85983400	1.44610900
C	-5.69848600	-3.74264700	2.03053300
H	-4.26332400	-2.16661500	2.24267700
C	-6.92234900	-2.98657800	2.53533800
H	-6.01538200	-4.49054400	1.28194300
H	-5.27401500	-4.32405200	2.86801800
C	-7.94654400	-3.88949000	3.21455000
H	-6.60039300	-2.20252000	3.24446200
H	-7.41172000	-2.45658400	1.70025300
H	-8.25888600	-4.67839200	2.50788500
H	-7.46469300	-4.41465300	4.05788600
C	-9.17289300	-3.13904100	3.71489700
H	-9.89156600	-3.81581000	4.20068500
H	-8.89534100	-2.36559800	4.44868700
H	-9.69724400	-2.63445900	2.88777900
C	9.17285700	-3.13906500	-3.71492400
H	9.69721500	-2.63449200	-2.88780500
H	9.89152400	-3.81583400	-4.20072100
H	8.89530500	-2.36561400	-4.44870700
H	4.26329800	-2.16662700	-2.24267700
C	-5.03041100	-1.99254200	0.25652200
C	-5.60831800	-2.74612600	-0.93604600
H	-4.15647300	-1.41094200	-0.07260300
H	-5.76877800	-1.25541000	0.61152800
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H	-4.89461000	-3.47574200	-1.34906800
H	-6.52874000	-3.29244200	-0.67836200
C	5.03039500	-1.99256700	-0.25652500
C	5.60830900	-2.74615900	0.93603500
H	4.15646000	-1.41096800	0.07261000
H	5.76876100	-1.25543400	-0.61153100
H	5.86060100	-2.04650800	1.74703400
H	4.89460400	-3.47577900	1.34905600
H	6.52873000	-3.29247300	0.67834100
C	-2.02112400	2.00034800	-1.72841500
C	-2.45330800	3.26265100	-2.07917300
S	-2.95898000	0.80669100	-2.61143500
C	-3.51167300	3.26814000	-3.03631100
O	-1.91506800	4.40383200	-1.57735800
C	-3.90361500	2.01780300	-3.43236900
O	-4.07517100	4.42115700	-3.49106800

C	-2.74390400	5.54425500	-1.81246100
C	-3.24701700	5.55465200	-3.23690300
H	-3.59176700	5.53388500	-1.10717600
H	-2.12144900	6.42451100	-1.61357200
H	-3.86723900	6.44057400	-3.41842300
H	-2.39687100	5.56086800	-3.94043300
C	2.02114000	2.00032900	1.72842400
C	2.45333600	3.26262900	2.07918000
S	2.95898500	0.80666500	2.61144500
C	3.51170100	3.26810900	3.03631900
O	1.91510700	4.40381500	1.57736500
C	3.90363100	2.01776900	3.43237800
O	4.07521000	4.42112100	3.49107500
C	2.74395400	5.54423000	1.81246700
C	3.24706600	5.55462300	3.23690900
H	3.59181700	5.53385200	1.10718300
H	2.12150700	6.42449200	1.61357700
H	3.86729700	6.44054000	3.41842900
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H	-5.32417200	2.57647500	-4.90826100
H	-4.62614600	0.95935000	-5.16692400
C	4.97984900	1.66550400	4.40105800
H	5.84913300	1.20563400	3.90444900
H	5.32419200	2.57642700	4.90826900
H	4.62615100	0.95930900	5.16693500
ii. Cation			
C	0.95559100	1.62582400	0.81411500
C	0.53166000	0.32881100	0.45253800
S	0.00001100	2.84925600	-0.00012000
C	-0.53161000	0.32874600	-0.45245100
O	1.13941800	-0.74897100	0.96868400
C	-0.95555800	1.62570800	-0.81419200
O	-1.13935800	-0.74911100	-0.96845400
C	0.30137400	-1.88733900	1.22954800
C	-0.30130700	-1.88751000	-1.22916800
H	0.84758600	-2.47203200	1.97982200
H	-0.64085100	-1.53671600	1.67322800
C	0.00003700	-2.75278500	0.00025000
H	-0.84751800	-2.47230800	-1.97936000
H	0.64091600	-1.53694200	-1.67289700
C	1.17375100	-3.66941400	-0.36307600
C	-1.17367900	-3.66935500	0.36370900
H	1.36937500	-4.36331200	0.47794300
H	0.89569900	-4.29354800	-1.23650500
O	2.31508100	-2.90734000	-0.65173600
H	-1.36922800	-4.36345500	-0.47716200
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C	5.71808700	-3.68204600	-1.99130100
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C	6.92568900	-2.90348000	-2.50120200
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H	7.41671400	-2.37316500	-1.66735500
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C	5.63521500	-2.69686400	0.97645200
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H	5.87969400	-1.99580900	1.78862700
H	4.94383800	-3.44576300	1.39276200
H	6.56545700	-3.21940400	0.70612700
C	-5.02847300	-1.95110500	0.20642900
C	-5.63508400	-2.69753100	-0.97643300
H	-4.14440700	-1.39071500	-0.13338700
H	-5.74669300	-1.19559700	0.56408200
H	-5.87955800	-1.99677500	-1.78886800
H	-4.94362000	-3.44652200	-1.39243400
H	-6.56530500	-3.22004900	-0.70599300
C	1.97089200	1.95229800	1.73067400
C	2.39652100	3.23819300	2.09516800
S	2.92262200	0.75457500	2.60105100
C	3.44225700	3.24332500	3.04300200
O	1.86035800	4.35183900	1.58501500
C	3.83929200	1.97823400	3.42341400
O	3.98477200	4.38414500	3.52586900
C	2.63171700	5.53275600	1.87757600
C	3.12810900	5.50792100	3.30344100
H	3.47208100	5.58361700	1.16889000
H	1.96029700	6.38159400	1.71025300
H	3.72668000	6.40183500	3.51121400
H	2.28094800	5.46834100	4.00732500
C	-1.97087100	1.95205100	-1.73078400
C	-2.39652100	3.23789300	-2.09543700
S	-2.92259800	0.75420300	-2.60099000
C	-3.44226400	3.24288900	-3.04326500
O	-1.86036900	4.35161200	-1.58543200
C	-3.83928300	1.97774400	-3.42351200
O	-3.98479600	4.38364000	-3.52627700
C	-2.63174600	5.53248200	-1.87814000
C	-3.12814700	5.50745600	-3.30399800
H	-3.47210500	5.58342300	-1.16945400
H	-1.96033500	6.38135000	-1.71093100

	H	-3.72673000	6.40133600	-3.51188300
	H	-2.28098900	5.46779600	-4.00788300
	C	4.91003800	1.63769100	4.39522000
	H	5.80945500	1.26644200	3.87900900
	H	5.18814000	2.53259600	4.96570800
	H	4.58435100	0.85579000	5.09534700
	C	-4.91002800	1.63706200	-4.39527300
	H	-5.80944000	1.26587200	-3.87901100
	H	-5.18813900	2.53188900	-4.96587700
	H	-4.58433300	0.85507300	-5.09529700
iii.	Dication			
	C	0.95013600	1.61080800	0.81186100
	C	0.52345100	0.28665700	0.44687400
	S	0.00004100	2.84831800	0.00011200
	C	-0.52352100	0.28674600	-0.44697700
	O	1.12682400	-0.76554100	0.98766500
	C	-0.95012500	1.61096900	-0.81179500
	O	-1.12695900	-0.76534300	-0.98789700
	C	0.29807300	-1.92497000	1.23466400
	C	-0.29828000	-1.92478300	-1.23511000
	H	0.85731300	-2.50534400	1.97697300
	H	-0.64235100	-1.57928700	1.68480800
	C	-0.00008900	-2.78144200	-0.00029000
	H	-0.85760200	-2.50502000	-1.97746500
	H	0.64213000	-1.57908100	-1.68526200
	C	1.17906200	-3.69106600	-0.36439000
	C	-1.17922100	-3.69113200	0.36368300
	H	1.37118600	-4.39125900	0.47162200
	H	0.91116500	-4.30718600	-1.24606700
	O	2.31295700	-2.91218900	-0.63433700
	H	-1.37136600	-4.39118100	-0.47244400
	H	-0.91129500	-4.30740300	1.24524600
	O	-2.31310300	-2.91229400	0.63379400
	C	3.42002500	-3.69317800	-1.05094100
	C	-3.42012700	-3.69333200	1.05042800
	H	3.68397200	-4.41918200	-0.25771100
	H	3.14210400	-4.28027000	-1.94720900
	H	-3.68415200	-4.41925300	0.25715000
	H	-3.14211200	-4.28051300	1.94660800
	C	-4.59688000	-2.78366900	1.37256000
	C	-5.73028800	-3.61927000	1.97785800
	C	-6.92806000	-2.81568300	2.47186500
	H	-6.07281600	-4.37256100	1.24634800
	H	-5.32075700	-4.19559900	2.82592300
	C	-7.97063900	-3.67201300	3.18255800
	H	-6.57807900	-2.02316700	3.15801900
	H	-7.41092500	-2.29423000	1.62772900
	H	-8.31105900	-4.46964900	2.49914200
	H	-7.49604500	-4.18848500	4.03517600
	C	4.59681100	-2.78348000	-1.37286200
	C	5.73031000	-3.61903300	-1.97805100
	H	4.24331700	-2.08808200	-2.15626400
	C	6.92814000	-2.81540700	-2.47185400
	H	6.07274700	-4.37236100	-1.24653700
	H	5.32090100	-4.19532000	-2.82620300
	C	7.97081700	-3.67168300	-3.18246800
	H	6.57824000	-2.02285100	-3.15800300
	H	7.41089300	-2.29400500	-1.62762300
	H	8.31115200	-4.46936400	-2.49906200
	H	7.49633900	-4.18810000	-4.03518400
	C	9.17151400	-2.87475000	-3.67287000
	H	9.90497000	-3.51955000	-4.17926100

H	8.86719400	-2.09267400	-4.38658500
H	9.68791700	-2.37550800	-2.83753400
C	-9.17127700	-2.87512100	3.67317100
H	-9.68779300	-2.37582600	2.83793600
H	-9.90466300	-3.51995900	4.17961500
H	-8.86686800	-2.09309000	4.38689800
H	-4.24328900	-2.08830600	2.15595100
C	5.01377900	-1.92347000	-0.16994600
C	5.63041900	-2.67687100	1.00321700
H	4.12139100	-1.37994700	0.17619400
H	5.72120000	-1.15333900	-0.51753700
H	5.86359900	-1.98434300	1.82596600
H	4.95076800	-3.44285100	1.40748700
H	6.56887500	-3.18048200	0.72604900
C	-5.01402600	-1.92360900	0.16974600
C	-5.63083700	-2.67696300	-1.00335800
H	-4.12168700	-1.38007400	-0.17650100
H	-5.72139500	-1.15349200	0.51747400
H	-5.86414000	-1.98440200	-1.82604500
H	-4.95124300	-3.44292600	-1.40775800
H	-6.56925100	-3.18058600	-0.72607200
C	1.94467800	1.91291500	1.71330800
C	2.38476300	3.21994100	2.08358000
S	2.90252700	0.70220700	2.57948800
C	3.42393300	3.21365000	3.01595500
O	1.86354000	4.31534500	1.56829100
C	3.80863400	1.92793100	3.38352100
O	3.97372600	4.33157000	3.51674100
C	2.62000500	5.51415100	1.88340100
C	3.12434500	5.46897500	3.30572800
H	3.44627600	5.58020800	1.16218600
H	1.92842600	6.34895500	1.73467400
H	3.73306800	6.35491800	3.51468400
H	2.28547400	5.42727500	4.01746500
C	-1.94465000	1.91326200	-1.71320100
C	-2.38464900	3.22037300	-2.08327200
S	-2.90258000	0.70274600	-2.57955900
C	-3.42382900	3.21429100	-3.01564100
O	-1.86334800	4.31566000	-1.56782100
C	-3.80861900	1.92865300	-3.38339700
O	-3.97354500	4.33232800	-3.51625100
C	-2.61970000	5.51457800	-1.88277800
C	-3.12405500	5.46962700	-3.30510600
H	-3.44595800	5.58062500	-1.16154700
H	-1.92804000	6.34929700	-1.73395300
H	-3.73269500	6.35565300	-3.51394600
H	-2.28519300	5.42793300	-4.01685500
C	4.87707700	1.59867000	4.35015200
H	5.85917000	1.79526100	3.88905300
H	4.79765100	2.25660600	5.22745100
H	4.84415600	0.55028700	4.66607000
C	-4.87712500	1.59962000	-4.35003400
H	-5.85920600	1.79541600	-3.88856200
H	-4.79819300	2.25821400	-5.22687700
H	-4.84381700	0.55146600	-4.66668300

b. EAE

i. Neutral

C	1.62260200	-1.32463800	-0.11743200
C	0.99347800	-0.09701300	-0.15190200
C	-0.40768400	-0.14945600	0.14957600
C	-0.85223900	-1.42497300	0.43188100

S	0.47276700	-2.56958600	0.29324500
O	-1.08874200	1.01330200	0.11755900
O	1.63951600	1.05379000	-0.48781800
C	-2.51013500	0.97275700	-0.04268400
C	-2.97757900	2.33189500	-0.54130500
H	-2.98078000	0.73302400	0.92361300
H	-2.76802800	0.17174500	-0.75358100
C	-4.50633000	2.40045200	-0.45427000
H	-2.57237500	3.07815000	0.16608500
C	-5.10534800	3.75603200	-0.81180100
H	-4.95421000	1.62158100	-1.09681000
H	-4.80681600	2.14286900	0.57636400
H	-4.61957900	4.54071800	-0.20399000
H	-4.88059600	4.00525200	-1.86301800
C	1.90682900	1.92360500	0.62742200
C	2.70795200	3.12167200	0.14179300
H	2.48319100	1.36191100	1.38187200
H	0.95080600	2.22919200	1.08281800
C	3.18494700	3.92971600	1.35414200
H	3.60486800	2.71083300	-0.35537200
C	4.11439000	5.09150500	1.02085600
H	2.31451200	4.30785100	1.91908400
H	3.71062000	3.24522200	2.04265700
H	4.96079300	4.71933700	0.41567300
H	3.59035700	5.82764700	0.38748800
C	-6.61444300	3.81827700	-0.60146300
C	-7.21684000	5.16911100	-0.96164700
H	-6.84418600	3.57966800	0.45178900
H	-7.09659100	3.02663300	-1.20150400
H	-8.30474300	5.18363100	-0.79830600
H	-6.77796100	5.97638100	-0.35389500
H	-7.03548800	5.41801200	-2.01938600
C	4.65398000	5.80074000	2.25832100
C	5.57928300	6.96402400	1.92963400
H	5.18812300	5.07055500	2.89125300
H	3.80646200	6.16292500	2.86638100
H	5.95269900	7.45427700	2.84104600
H	6.45378500	6.62684200	1.35062800
H	5.06170400	7.72846200	1.32844700
C	-2.40466300	2.66421500	-1.92809800
C	-2.94653500	1.83278100	-3.08576700
H	-1.31143200	2.54456900	-1.87492400
H	-2.57882400	3.73208700	-2.13652800
H	-2.44428800	2.10907100	-4.02484000
H	-2.78176700	0.75434000	-2.93687900
H	-4.02616900	1.98497300	-3.23684100
C	1.94971100	3.94680700	-0.90943300
C	0.75253700	4.73573400	-0.39174300
H	1.61988200	3.25738800	-1.70240900
H	2.65832400	4.63919700	-1.39216200
H	0.23607400	5.24143500	-1.22121900
H	0.01410000	4.08709300	0.10325200
H	1.04919000	5.51237800	0.32960300
C	-2.14588800	-1.92537900	0.88102000
C	-3.15140500	-2.49878700	0.14301200
S	-2.59412200	-1.93135500	2.57627400
C	-4.26867500	-2.92709900	0.92868200
O	-3.10895700	-2.63712700	-1.20468600
C	-4.12665400	-2.69174900	2.27051100
O	-5.36936800	-3.50587400	0.37375900
C	-4.38618200	-2.95535000	-1.76401500
C	-5.09787400	-3.99958300	-0.93697800

H	-4.99743300	-2.03954900	-1.82737000
H	-4.19394100	-3.32735800	-2.77739900
H	-6.06783800	-4.24725700	-1.38429200
H	-4.48783600	-4.91683300	-0.87112600
C	3.00272200	-1.62264400	-0.41079300
C	3.64221200	-2.84180100	-0.33572000
S	4.14407300	-0.40288200	-0.94531000
C	5.02290600	-2.79299900	-0.69476900
O	3.02232000	-3.99063700	0.02891300
C	5.45427200	-1.54367000	-1.05106800
O	5.82051800	-3.89551900	-0.66861600
C	3.94720400	-5.03160700	0.35609200
C	5.05805500	-5.10170100	-0.66504800
H	4.36145000	-4.84978400	1.36164400
H	3.37004900	-5.96346200	0.36795000
H	5.75568300	-5.91058800	-0.41750900
H	4.64081500	-5.28188200	-1.67051500
C	-5.10390500	-3.00355700	3.35249100
H	-4.62655800	-3.52463800	4.19499900
H	-5.57985300	-2.09419500	3.75166500
H	-5.89531200	-3.65040500	2.95138900
C	6.82684300	-1.14233100	-1.47011900
H	6.81302300	-0.54336200	-2.39249700
H	7.33612400	-0.54617700	-0.69642200
H	7.42892400	-2.04198500	-1.65341900
ii. Cation			
C	0.06276800	1.68479600	-0.20398600
C	-0.43569700	0.39435500	0.10528100
C	0.57215600	-0.52906100	0.40691800
C	1.85563900	0.06294600	0.46630300
S	1.80575300	1.73428600	-0.05790300
O	0.32898900	-1.83007700	0.67255600
O	-1.75224700	0.17001800	0.04591100
C	0.82210700	-2.81316200	-0.28044200
C	-0.26658400	-3.36666500	-1.19022500
H	1.22982200	-3.62283800	0.33845800
H	1.65261800	-2.37384000	-0.85373400
C	0.26278600	-4.66106600	-1.82638400
H	-1.10802200	-3.64903700	-0.53213800
C	-0.74719100	-5.40923500	-2.68938300
H	1.16525700	-4.44405700	-2.42486200
H	0.59821400	-5.33201300	-1.01669900
H	-1.67449700	-5.56958300	-2.11025500
H	-1.03477700	-4.79451300	-3.55918400
C	-2.35344800	-0.67505900	1.06191600
C	-3.82636200	-0.32101400	1.17846200
H	-1.83150200	-0.48905900	2.01234600
H	-2.20052400	-1.72646900	0.78461800
C	-4.40793000	-1.05676400	2.39266200
H	-3.87191700	0.76114900	1.39392600
C	-5.85529600	-0.70198300	2.71521600
H	-4.32152000	-2.14799300	2.24799300
H	-3.78400300	-0.82294600	3.27274700
H	-5.95015300	0.39504300	2.80675600
H	-6.51358000	-0.99474700	1.87958800
C	-0.22515700	-6.75302400	-3.18710800
C	-1.22634800	-7.50100500	-4.05619800
H	0.05265300	-7.37812900	-2.32056700
H	0.70845400	-6.59130900	-3.75389500
H	-0.82287100	-8.46556100	-4.39822900
H	-2.15799000	-7.70610300	-3.50529400
H	-1.49444700	-6.91616500	-4.95039600

C	-6.35968900	-1.36011400	3.99507700
C	-7.80596100	-1.01287800	4.31893900
H	-5.71005700	-1.06237100	4.83665200
H	-6.25348800	-2.45538900	3.90514200
H	-8.14036100	-1.50019800	5.24676100
H	-7.93633200	0.07341200	4.44749000
H	-8.48390400	-1.33266200	3.51170200
C	-0.79898000	-2.34933000	-2.21007500
C	0.19442300	-1.88709100	-3.27041500
H	-1.18903100	-1.47478600	-1.66810700
H	-1.67748700	-2.78992400	-2.70788400
H	-0.27373100	-1.14716900	-3.93614100
H	1.08331800	-1.40807200	-2.83147700
H	0.54397300	-2.71831900	-3.90110100
C	-4.59536100	-0.55711800	-0.13104900
C	-4.77525100	-2.01390200	-0.54232500
H	-4.07786000	-0.01119900	-0.93564000
H	-5.58502900	-0.08130600	-0.04237500
H	-5.29144100	-2.07744400	-1.51158700
H	-3.81360700	-2.53783500	-0.65354000
H	-5.37734300	-2.57852400	0.18541300
C	3.04850700	-0.50718900	0.95675100
C	4.33525800	0.04538800	0.90481200
S	3.10272400	-2.01611800	1.85925200
C	5.31448900	-0.72964600	1.56574700
O	4.60570900	1.20044700	0.28901400
C	4.80855100	-1.87635600	2.13972000
O	6.61418800	-0.36107600	1.63071000
C	6.01693200	1.44267200	0.13057900
C	6.77439900	1.03687100	1.37189000
H	6.36886600	0.87920400	-0.74666600
H	6.11933000	2.51626000	-0.05983300
H	7.84772100	1.20708600	1.23270700
H	6.42657100	1.61334000	2.24452300
C	-0.68660600	2.80788400	-0.59210600
C	-0.18795900	4.08149500	-0.91409000
S	-2.44156100	2.82037300	-0.72546300
C	-1.18827500	5.01442200	-1.25620700
O	1.11522000	4.37497900	-0.89247400
C	-2.46322100	4.48860000	-1.20562600
O	-0.90909600	6.28992200	-1.60662000
C	1.37769900	5.78891500	-0.98602000
C	0.46013300	6.43828800	-1.99412500
H	1.24346300	6.23261400	0.01190400
H	2.42553300	5.88209600	-1.29034600
H	0.65505600	7.51525700	-2.04421700
H	0.60780500	5.99682300	-2.99301400
C	5.56733200	-2.89875200	2.90526100
H	5.02658200	-3.20889100	3.80997800
H	5.74139500	-3.80011400	2.29664300
H	6.54297700	-2.48985800	3.19631600
C	-3.73041200	5.20467200	-1.50034300
H	-4.41709900	4.58234200	-2.09034600
H	-4.25102900	5.48334400	-0.57029500
H	-3.51344400	6.12474800	-2.05736600
iii. Dication			
C	0.39298200	1.65649500	-0.21212600
C	-0.34962200	0.45810000	0.13163700
C	0.46899600	-0.62898600	0.36553100
C	1.86050700	-0.25885500	0.41013400
S	2.12416800	1.38892800	-0.14951400
O	0.03806600	-1.87218700	0.61890300

O	-1.66618900	0.53737900	0.15110800
C	0.31629700	-2.90521800	-0.38479400
C	-0.87615800	-3.21063900	-1.27816000
H	0.57189800	-3.79110300	0.20907900
H	1.20392700	-2.60906600	-0.96378400
C	-0.61696800	-4.56836300	-1.95098300
H	-1.74309100	-3.34408800	-0.60678000
C	-1.76893900	-5.08526400	-2.80574800
H	0.29975500	-4.51589300	-2.56419200
H	-0.40526100	-5.30973300	-1.16154000
H	-2.69965500	-5.07234000	-2.21053200
H	-1.94402000	-4.40926400	-3.65974900
C	-2.43520000	-0.35071400	1.02188900
C	-3.79460700	0.27989100	1.26000800
H	-1.87354600	-0.45801200	1.96001800
H	-2.50621200	-1.33240600	0.53738100
C	-4.49203100	-0.49422600	2.38713700
H	-3.60391600	1.30212200	1.63188200
C	-5.82435100	0.10122600	2.82910000
H	-4.64130100	-1.54552600	2.08531400
H	-3.81496800	-0.52658200	3.25808900
H	-5.68143900	1.16743400	3.08083900
H	-6.54596400	0.07988100	1.99493400
C	-1.52802300	-6.49523500	-3.33498300
C	-2.67039800	-7.01482100	-4.19631500
H	-1.36486300	-7.17925400	-2.48402400
H	-0.58996600	-6.50818200	-3.91698800
H	-2.46933800	-8.03286200	-4.56105100
H	-3.61522400	-7.04404300	-3.63080000
H	-2.83226100	-6.37171200	-5.07584600
C	-6.43084700	-0.62323300	4.02614700
C	-7.76304100	-0.03578400	4.47011800
H	-5.71573500	-0.59676900	4.86680100
H	-6.56215400	-1.69024100	3.77505400
H	-8.17430200	-0.57728800	5.33471500
H	-7.65637900	1.02177500	4.75928600
H	-8.50971400	-0.08285500	3.66166100
C	-1.21912800	-2.08761600	-2.26831400
C	-0.17523900	-1.80236500	-3.34218100
H	-1.42762800	-1.16306700	-1.70821400
H	-2.17465100	-2.34161000	-2.75331600
H	-0.50600000	-0.97339100	-3.98457500
H	0.79831800	-1.51193000	-2.91764100
H	-0.00554500	-2.67241700	-3.99358900
C	-4.62266200	0.40348200	-0.02900100
C	-5.13285900	-0.90559800	-0.62007800
H	-4.01587800	0.93112800	-0.78230800
H	-5.47798200	1.06695700	0.17393800
H	-5.66952000	-0.71533900	-1.56093100
H	-4.31747800	-1.60821500	-0.85081700
H	-5.83184500	-1.42009700	0.05587800
C	2.89629000	-1.01967300	0.90958200
C	4.27978100	-0.67251700	0.92206700
S	2.67175400	-2.55598400	1.75809900
C	5.08203700	-1.60366200	1.58875800
O	4.74206200	0.41858000	0.34636800
C	4.35668100	-2.67221100	2.10197600
O	6.40836200	-1.45532400	1.74087100
C	6.19204200	0.47901700	0.29064600
C	6.80081400	-0.08815900	1.54996000
H	6.50876000	-0.07991300	-0.60053300
H	6.43981500	1.53837200	0.17239600

H	7.89292100	-0.08565800	1.47099500
H	6.49764800	0.49857100	2.43100800
C	-0.15243000	2.87171900	-0.54946400
C	0.57546300	4.04765400	-0.91804400
S	-1.88624800	3.22961900	-0.56230100
C	-0.24060100	5.14389600	-1.19890500
O	1.89052900	4.07643300	-0.96727700
C	-1.59390600	4.85717600	-1.04982500
O	0.23452700	6.33691700	-1.58999700
C	2.43388100	5.41381100	-1.13418100
C	1.57917700	6.22346900	-2.07903400
H	2.48357000	5.87234000	-0.13708800
H	3.44390300	5.27537200	-1.53153300
H	1.97001100	7.24342600	-2.15521300
H	1.55878800	5.76499400	-3.07963500
C	4.92155200	-3.80627700	2.86386500
H	4.16811200	-4.30335900	3.48547900
H	5.33061200	-4.55073000	2.16031400
H	5.75366200	-3.45557500	3.48903900
C	-2.69787400	5.81552300	-1.26307700
H	-3.66784600	5.31702200	-1.36590900
H	-2.74984800	6.50560900	-0.40430600
H	-2.49152600	6.42583600	-2.15359700

c. **EAAE**

i. Neutral

C	-1.54311300	2.76718900	-1.04796900
C	-0.38335800	3.03146600	-0.34778300
C	0.35241800	1.86078400	0.02887100
C	-0.24124300	0.68663800	-0.39460200
S	-1.72546900	1.04562300	-1.26462100
O	1.49742300	2.04259100	0.72109500
O	-0.00235700	4.29265700	-0.00418500
C	1.91226500	1.04224300	1.65888000
C	2.77292800	1.70414400	2.72519400
H	2.48610300	0.26377100	1.13338600
H	1.02088700	0.56663600	2.09689000
C	3.45674700	0.61888700	3.56419500
H	3.56587000	2.25084700	2.18285700
C	4.45220800	1.14162500	4.59384500
H	2.69496800	0.00150100	4.07274400
H	3.98523600	-0.06745800	2.87978200
H	5.18568100	1.79777900	4.09120000
H	3.93546900	1.77670500	5.33371300
C	1.08634600	4.80688600	-0.79415300
C	1.33392000	6.25983100	-0.41896800
H	0.81219300	4.73244400	-1.86001400
H	1.97879100	4.18269600	-0.62459900
C	2.32350600	6.87280900	-1.41685000
H	0.36832500	6.77991400	-0.55030500
C	2.56337500	8.36805400	-1.23940200
H	3.28873100	6.33850600	-1.36510500
H	1.94139400	6.69679900	-2.43757200
H	1.59261400	8.89601600	-1.24428300
H	3.01055200	8.56646700	-0.25028500
C	5.19227900	0.02925300	5.32900100
C	6.18465800	0.54650600	6.36098400
H	5.71920200	-0.60361400	4.59357100
H	4.45679500	-0.63068600	5.82164900
H	6.70286800	-0.27801700	6.87288500
H	6.95245600	1.18256300	5.89236500
H	5.68085200	1.15228900	7.13096400

C	3.46478300	8.96196700	-2.31654600
C	3.70971100	10.45410800	-2.14056200
H	3.01700900	8.77497500	-3.30831600
H	4.43032800	8.42631500	-2.31640500
H	4.36139200	10.85346800	-2.93193900
H	2.76476400	11.01968400	-2.17023600
H	4.19100300	10.66840000	-1.17303600
C	1.98827900	2.74117100	3.54357100
C	0.93450500	2.18097200	4.49248100
H	1.50808800	3.43100800	2.83271200
H	2.70294500	3.35238500	4.11782800
H	0.39677900	2.99910200	4.99451700
H	0.18042700	1.57454600	3.96721000
H	1.37611300	1.55033700	5.27907300
C	1.73797000	6.42654300	1.05398500
C	3.12945400	5.92189300	1.41837800
H	0.98573100	5.90825200	1.66919900
H	1.65834600	7.49244100	1.32239200
H	3.30459000	6.02074900	2.50001400
H	3.26425400	4.85982700	1.16344500
H	3.92190100	6.48886400	0.90651200
C	-2.53160500	3.70486800	-1.51766900
C	-3.66541600	3.44207800	-2.25734900
S	-2.43659700	5.42671200	-1.19681000
C	-4.43740000	4.60276000	-2.56346100
O	-4.02997000	2.19739400	-2.65034100
C	-3.90906900	5.76199700	-2.06221700
O	-5.58269800	4.54205300	-3.29597000
C	-5.03029300	2.21753900	-3.67296900
C	-6.11281300	3.21799800	-3.34318600
H	-4.56003400	2.46530600	-4.63899100
H	-5.44030500	1.20217000	-3.72220100
H	-6.88408900	3.21873500	-4.12257600
H	-6.58013900	2.96889600	-2.37517100
C	-4.45220800	7.14234800	-2.20396300
H	-4.49507700	7.66529900	-1.23730000
H	-3.84289100	7.75679400	-2.88553000
H	-5.46973800	7.09241100	-2.61335400
C	0.24124300	-0.68663800	-0.39460200
C	-0.35241800	-1.86078400	0.02887100
S	1.72546900	-1.04562300	-1.26462100
C	0.38335800	-3.03146600	-0.34778300
O	-1.49742300	-2.04259100	0.72109500
C	1.54311300	-2.76718900	-1.04796900
O	0.00235700	-4.29265700	-0.00418500
C	-1.91226500	-1.04224300	1.65888000
C	2.53160500	-3.70486800	-1.51766900
C	-1.08634600	-4.80688600	-0.79415300
C	-2.77292800	-1.70414400	2.72519400
H	-2.48610300	-0.26377100	1.13338600
H	-1.02088700	-0.56663600	2.09689000
C	3.66541600	-3.44207800	-2.25734900
S	2.43659700	-5.42671200	-1.19681000
C	-1.33392000	-6.25983100	-0.41896800
H	-0.81219300	-4.73244400	-1.86001400
H	-1.97879100	-4.18269600	-0.62459900
C	-3.45674700	-0.61888700	3.56419500
H	-3.56587000	-2.25084700	2.18285700
C	-1.98827900	-2.74117100	3.54357100
C	4.43740000	-4.60276000	-2.56346100
O	4.02997000	-2.19739400	-2.65034100
C	3.90906900	-5.76199700	-2.06221700

C	-2.32350600	-6.87280900	-1.41685000
H	-0.36832500	-6.77991400	-0.55030500
C	-1.73797000	-6.42654300	1.05398500
C	-4.45220800	-1.14162500	4.59384500
H	-2.69496800	-0.00150100	4.07274400
H	-3.98523600	0.06745800	2.87978200
C	-0.93450500	-2.18097200	4.49248100
H	-1.50808800	-3.43100800	2.83271200
H	-2.70294500	-3.35238500	4.11782800
O	5.58269800	-4.54205300	-3.29597000
C	5.03029300	-2.21753900	-3.67296900
C	4.45220800	-7.14234800	-2.20396300
C	-2.56337500	-8.36805400	-1.23940200
H	-3.28873100	-6.33850600	-1.36510500
H	-1.94139400	-6.69679900	-2.43757200
C	-3.12945400	-5.92189300	1.41837800
H	-0.98573100	-5.90825200	1.66919900
H	-1.65834600	-7.49244100	1.32239200
H	-5.18568100	-1.79777900	4.09120000
H	-3.93546900	-1.77670500	5.33371300
C	-5.19227900	-0.02925300	5.32900100
H	-0.39677900	-2.99910200	4.99451700
H	-0.18042700	-1.57454600	3.96721000
H	-1.37611300	-1.55033700	5.27907300
C	6.11281300	-3.21799800	-3.34318600
H	4.56003400	-2.46530600	-4.63899100
H	5.44030500	-1.20217000	-3.72220100
H	4.49507700	-7.66529900	-1.23730000
H	3.84289100	-7.75679400	-2.88553000
H	5.46973800	-7.09241100	-2.61335400
H	-1.59261400	-8.89601600	-1.24428300
H	-3.01055200	-8.56646700	-0.25028500
C	-3.46478300	-8.96196700	-2.31654600
H	-3.30459000	-6.02074900	2.50001400
H	-3.26425400	-4.85982700	1.16344500
H	-3.92190100	-6.48886400	0.90651200
C	-6.18465800	-0.54650600	6.36098400
H	-5.71920200	0.60361400	4.59357100
H	-4.45679500	0.63068600	5.82164900
H	6.88408900	-3.21873500	-4.12257600
H	6.58013900	-2.96889600	-2.37517100
C	-3.70971100	-10.45410800	-2.14056200
H	-3.01700900	-8.77497500	-3.30831600
H	-4.43032800	-8.42631500	-2.31640500
H	-6.70286800	0.27801700	6.87288500
H	-6.95245600	-1.18256300	5.89236500
H	-5.68085200	-1.15228900	7.13096400
H	-4.36139200	-10.85346800	-2.93193900
H	-2.76476400	-11.01968400	-2.17023600
H	-4.19100300	-10.66840000	-1.17303600
ii. Cation			
C	-1.88173500	2.53403500	-0.66124200
C	-0.56569300	2.95527700	-0.39278300
C	0.29872200	1.90111800	-0.06162000
C	-0.31241400	0.63212100	-0.16141600
S	-2.02020800	0.79860800	-0.53288100
O	1.58919800	2.10666100	0.26670200
O	-0.24769500	4.26433200	-0.40917500
C	2.03800700	1.67171500	1.57844300
C	2.29689900	2.84626500	2.51118800
H	2.97191800	1.12110300	1.40372900
H	1.30179000	0.96918000	1.99737200

C	3.06608100	2.32513900	3.73324300
H	2.97120900	3.53082200	1.96621900
C	3.51330900	3.40446700	4.71290500
H	2.45737100	1.57519100	4.26877600
H	3.95867200	1.78242000	3.37622500
H	4.07190300	4.18527300	4.16591100
H	2.63466600	3.90922600	5.14931400
C	0.84474400	4.64229700	-1.28452800
C	0.85251600	6.15406800	-1.44001600
H	0.68185100	4.15892500	-2.26076500
H	1.78568300	4.26299700	-0.86110600
C	1.88173500	6.52833000	-2.51423200
H	-0.14344100	6.43354200	-1.82634000
C	1.91054400	8.00889100	-2.87742600
H	2.88983100	6.20944600	-2.19581000
H	1.66033200	5.94684900	-3.42612900
H	0.89068800	8.33857300	-3.14595000
H	2.20192000	8.60985800	-1.99916400
C	4.38172000	2.86134800	5.84280000
C	4.82448800	3.93378200	6.82822500
H	5.26904200	2.36507400	5.41232800
H	3.82594700	2.07261300	6.37951200
H	5.44955800	3.51278300	7.62961500
H	5.41111400	4.71941000	6.32604200
H	3.95860100	4.42208800	7.30287400
C	2.86089200	8.32313700	-4.02792700
C	2.89742500	9.80120100	-4.39017400
H	2.56714800	7.73221400	-4.91308400
H	3.87681700	7.98237800	-3.76173300
H	3.58921900	9.99625400	-5.22299500
H	1.90169400	10.16260300	-4.69261200
H	3.22430600	10.41399500	-3.53509800
C	1.02752500	3.63695200	2.85787200
C	-0.01112600	2.89726200	3.69397900
H	0.56760600	3.98154700	1.91908600
H	1.32708100	4.55623200	3.38603700
H	-0.88975300	3.53649900	3.86549000
H	-0.37175200	1.98144700	3.20001300
H	0.37971500	2.60841700	4.68140000
C	1.04045100	6.88725500	-0.10294600
C	2.41745500	6.75538200	0.53694500
H	0.27358800	6.52094300	0.59757100
H	0.81373400	7.95441700	-0.25675800
H	2.43746800	7.25976200	1.51434700
H	2.69643800	5.70456800	0.70840200
H	3.20645600	7.20998700	-0.08100000
C	-2.99295600	3.35117700	-0.97390300
C	-4.30157800	2.93183600	-1.22317500
S	-2.90444900	5.10102200	-1.12167600
C	-5.19311300	3.98990800	-1.51975000
O	-4.67531700	1.64504000	-1.18432000
C	-4.59297000	5.22863700	-1.50419400
O	-6.50570800	3.78466500	-1.78349000
C	-5.98346400	1.42133700	-1.74036600
C	-6.94089200	2.50724300	-1.31142400
H	-5.89681400	1.38646800	-2.83717100
H	-6.30727200	0.44308000	-1.36892500
H	-7.93082300	2.33397900	-1.74819200
H	-7.02976500	2.53158200	-0.21289100
C	-5.24358100	6.53782200	-1.77490600
H	-4.92682600	7.30317800	-1.05282800
H	-4.99281400	6.90746000	-2.78177200

H	-6.33364100	6.42559100	-1.71619400
C	0.31241400	-0.63212100	-0.16141600
C	-0.29872200	-1.90111800	-0.06162000
S	2.02020800	-0.79860800	-0.53288100
C	0.56569300	-2.95527700	-0.39278300
O	-1.58919800	-2.10666100	0.26670200
C	1.88173500	-2.53403500	-0.66124200
O	0.24769500	-4.26433200	-0.40917500
C	-2.03800700	-1.67171500	1.57844300
C	2.99295600	-3.35117700	-0.97390300
C	-0.84474400	-4.64229700	-1.28452800
C	-2.29689900	-2.84626500	2.51118800
H	-2.97191800	-1.12110300	1.40372900
H	-1.30179000	-0.96918000	1.99737200
C	4.30157800	-2.93183600	-1.22317500
S	2.90444900	-5.10102200	-1.12167600
C	-0.85251600	-6.15406800	-1.44001600
H	-0.68185100	-4.15892500	-2.26076500
H	-1.78568300	-4.26299700	-0.86110600
C	-3.06608100	-2.32513900	3.73324300
H	-2.97120900	-3.53082200	1.96621900
C	-1.02752500	-3.63695200	2.85787200
C	5.19311300	-3.98990800	-1.51975000
O	4.67531700	-1.64504000	-1.18432000
C	4.59297000	-5.22863700	-1.50419400
C	-1.88173500	-6.52833000	-2.51423200
H	0.14344100	-6.43354200	-1.82634000
C	-1.04045100	-6.88725500	-0.10294600
C	-3.51330900	-3.40446700	4.71290500
H	-2.45737100	-1.57519100	4.26877600
H	-3.95867200	-1.78242000	3.37622500
C	0.01112600	-2.89726200	3.69397900
H	-0.56760600	-3.98154700	1.91908600
H	-1.32708100	-4.55623200	3.38603700
O	6.50570800	-3.78466500	-1.78349000
C	5.98346400	-1.42133700	-1.74036600
C	5.24358100	-6.53782200	-1.77490600
C	-1.91054400	-8.00889100	-2.87742600
H	-2.88983100	-6.20944600	-2.19581000
H	-1.66033200	-5.94684900	-3.42612900
C	-2.41745500	-6.75538200	0.53694500
H	-0.27358800	-6.52094300	0.59757100
H	-0.81373400	-7.95441700	-0.25675800
H	-4.07190300	-4.18527300	4.16591100
H	-2.63466600	-3.90922600	5.14931400
C	-4.38172000	-2.86134800	5.84280000
H	0.88975300	-3.53649900	3.86549000
H	0.37175200	-1.98144700	3.20001300
H	-0.37971500	-2.60841700	4.68140000
C	6.94089200	-2.50724300	-1.31142400
H	5.89681400	-1.38646800	-2.83717100
H	6.30727200	-0.44308000	-1.36892500
H	4.92682600	-7.30317800	-1.05282800
H	4.99281400	-6.90746000	-2.78177200
H	6.33364100	-6.42559100	-1.71619400
H	-0.89068800	-8.33857300	-3.14595000
H	-2.20192000	-8.60985800	-1.99916400
C	-2.86089200	-8.32313700	-4.02792700
H	-2.43746800	-7.25976200	1.51434700
H	-2.69643800	-5.70456800	0.70840200
H	-3.20645600	-7.20998700	-0.08100000
C	-4.82448800	-3.93378200	6.82822500

H	-5.26904200	-2.36507400	5.41232800
H	-3.82594700	-2.07261300	6.37951200
H	7.93082300	-2.33397900	-1.74819200
H	7.02976500	-2.53158200	-0.21289100
C	-2.89742500	-9.80120100	-4.39017400
H	-2.56714800	-7.73221400	-4.91308400
H	-3.87681700	-7.98237800	-3.76173300
H	-5.44955800	-3.51278300	7.62961500
H	-5.41111400	-4.71941000	6.32604200
H	-3.95860100	-4.42208800	7.30287400
H	-3.58921900	-9.99625400	-5.22299500
H	-1.90169400	-10.16260300	-4.69261200
H	-3.22430600	-10.41399500	-3.53509800
iii. Dication			
C	-1.99163100	2.40262800	-0.54839200
C	-0.65813200	2.90189200	-0.36208800
C	0.23824400	1.91580400	0.01140500
C	-0.33885700	0.60050700	-0.01829400
S	-2.07943100	0.67927600	-0.29548600
O	1.52535300	2.14679800	0.30498000
O	-0.44088200	4.20574100	-0.51537800
C	1.98263600	1.86432700	1.66547600
C	2.14578100	3.12643400	2.49874400
H	2.95588400	1.37490400	1.53446900
H	1.29359700	1.14461900	2.13248500
C	2.98609700	2.76783900	3.73407200
H	2.74556100	3.82547200	1.88897200
C	3.34346200	3.95174900	4.62599900
H	2.46490900	2.00137900	4.33419500
H	3.92073300	2.29198800	3.39040600
H	3.80700000	4.74470300	4.01197700
H	2.42908400	4.39491500	5.05549900
C	0.82498000	4.64388200	-1.08665500
C	0.63290400	6.02968900	-1.67678100
H	1.11088800	3.92062500	-1.86418700
H	1.58865800	4.62950500	-0.29821600
C	1.88889500	6.39096200	-2.48097300
H	-0.20529000	5.95216000	-2.39160100
C	1.79512400	7.70994000	-3.24015500
H	2.76877100	6.41288200	-1.81442300
H	2.08343300	5.58114300	-3.20535700
H	0.88524900	7.70602300	-3.86688400
H	1.67296500	8.54768000	-2.53276600
C	4.28911500	3.57530100	5.76178300
C	4.64283200	4.75104700	6.66150500
H	5.21197600	3.14279400	5.33746500
H	3.82929500	2.77296100	6.36488000
H	5.32660700	4.44974100	7.46872100
H	5.13390500	5.55587300	6.09187100
H	3.74309700	5.18043800	7.12995300
C	3.01195100	7.97899700	-4.11909300
C	2.92563200	9.29704400	-4.87562700
H	3.13301900	7.14788900	-4.83569200
H	3.92044800	7.97125500	-3.49179300
H	3.81543100	9.46255100	-5.50081900
H	2.04482100	9.32080200	-5.53672600
H	2.84138400	10.14997400	-4.18368400
C	0.81813500	3.82321600	2.83071900
C	-0.12915500	3.05443700	3.74505100
H	0.30034000	4.06979700	1.89094200
H	1.04937200	4.79767000	3.28888100
H	-1.05488000	3.62669700	3.90311500

H	-0.42175100	2.07959200	3.32480900
H	0.31254800	2.86827600	4.73532300
C	0.23824400	7.07224500	-0.61857400
C	1.32333300	7.44343200	0.38561900
H	-0.64626100	6.69803900	-0.07891900
H	-0.09944900	7.98213400	-1.13948500
H	0.93065700	8.15426400	1.12735600
H	1.69554600	6.56943900	0.94174900
H	2.18866900	7.92120500	-0.09761100
C	-3.10781800	3.15799000	-0.88623900
C	-4.42894300	2.67359300	-1.04840600
S	-3.07909900	4.89304900	-1.20891200
C	-5.35317800	3.66719200	-1.40394500
O	-4.74625200	1.39754300	-0.88792700
C	-4.77575100	4.92016200	-1.52726500
O	-6.66502200	3.41933100	-1.58554200
C	-6.08629800	1.07796500	-1.33453600
C	-7.04925800	2.18257600	-0.97220300
H	-6.04768300	0.92068600	-2.42177500
H	-6.35188500	0.14117100	-0.83457800
H	-8.05019000	1.94532200	-1.34834900
H	-7.09440000	2.31818900	0.11989000
C	-5.48273200	6.16850800	-1.89834200
H	-4.96447500	7.05969300	-1.52466600
H	-5.55081900	6.24982200	-2.99559100
H	-6.50795100	6.14589900	-1.50535700
C	0.33885700	-0.60050700	-0.01829400
C	-0.23824400	-1.91580400	0.01140500
S	2.07943100	-0.67927600	-0.29548600
C	0.65813200	-2.90189200	-0.36208800
O	-1.52535300	-2.14679800	0.30498000
C	1.99163100	-2.40262800	-0.54839200
O	0.44088200	-4.20574100	-0.51537800
C	-1.98263600	-1.86432700	1.66547600
C	3.10781800	-3.15799000	-0.88623900
C	-0.82498000	-4.64388200	-1.08665500
C	-2.14578100	-3.12643400	2.49874400
H	-2.95588400	-1.37490400	1.53446900
H	-1.29359700	-1.14461900	2.13248500
C	4.42894300	-2.67359300	-1.04840600
S	3.07909900	-4.89304900	-1.20891200
C	-0.63290400	-6.02968900	-1.67678100
H	-1.11088800	-3.92062500	-1.86418700
H	-1.58865800	-4.62950500	-0.29821600
C	-2.98609700	-2.76783900	3.73407200
H	-2.74556100	-3.82547200	1.88897200
C	-0.81813500	-3.82321600	2.83071900
C	5.35317800	-3.66719200	-1.40394500
O	4.74625200	-1.39754300	-0.88792700
C	4.77575100	-4.92016200	-1.52726500
C	-1.88889500	-6.39096200	-2.48097300
H	0.20529000	-5.95216000	-2.39160100
C	-0.23824400	-7.07224500	-0.61857400
C	-3.34346200	-3.95174900	4.62599900
H	-2.46490900	-2.00137900	4.33419500
H	-3.92073300	-2.29198800	3.39040600
C	0.12915500	-3.05443700	3.74505100
H	-0.30034000	-4.06979700	1.89094200
H	-1.04937200	-4.79767000	3.28888100
O	6.66502200	-3.41933100	-1.58554200
C	6.08629800	-1.07796500	-1.33453600
C	5.48273200	-6.16850800	-1.89834200

C	-1.79512400	-7.70994000	-3.24015500
H	-2.76877100	-6.41288200	-1.81442300
H	-2.08343300	-5.58114300	-3.20535700
C	-1.32333300	-7.44343200	0.38561900
H	0.64626100	-6.69803900	-0.07891900
H	0.09944900	-7.98213400	-1.13948500
H	-3.80700000	-4.74470300	4.01197700
H	-2.42908400	-4.39491500	5.05549900
C	-4.28911500	-3.57530100	5.76178300
H	1.05488000	-3.62669700	3.90311500
H	0.42175100	-2.07959200	3.32480900
H	-0.31254800	-2.86827600	4.73532300
C	7.04925800	-2.18257600	-0.97220300
H	6.04768300	-0.92068600	-2.42177500
H	6.35188500	-0.14117100	-0.83457800
H	4.96447500	-7.05969300	-1.52466600
H	5.55081900	-6.24982200	-2.99559100
H	6.50795100	-6.14589900	-1.50535700
H	-0.88524900	-7.70602300	-3.86688400
H	-1.67296500	-8.54768000	-2.53276600
C	-3.01195100	-7.97899700	-4.11909300
H	-0.93065700	-8.15426400	1.12735600
H	-1.69554600	-6.56943900	0.94174900
H	-2.18866900	-7.92120500	-0.09761100
C	-4.64283200	-4.75104700	6.66150500
H	-5.21197600	-3.14279400	5.33746500
H	-3.82929500	-2.77296100	6.36488000
H	8.05019000	-1.94532200	-1.34834900
H	7.09440000	-2.31818900	0.11989000
C	-2.92563200	-9.29704400	-4.87562700
H	-3.13301900	-7.14788900	-4.83569200
H	-3.92044800	-7.97125500	-3.49179300
H	-5.32660700	-4.44974100	7.46872100
H	-5.13390500	-5.55587300	6.09187100
H	-3.74309700	-5.18043800	7.12995300
H	-3.81543100	-9.46255100	-5.50081900
H	-2.04482100	-9.32080200	-5.53672600
H	-2.84138400	-10.14997400	-4.18368400

d. **EABAE**

i. Neutral

C	0.72735500	0.50299000	0.73396800
C	-0.66692300	0.54176100	0.74932000
C	-1.43227200	0.09745200	-0.33693400
C	-0.76746000	-0.38989700	-1.47964800
C	0.62670500	-0.42316600	-1.49730900
C	1.39320700	0.02236400	-0.41154800
H	-1.19643900	0.90643500	1.62796600
H	1.15527300	-0.78263900	-2.37877000
O	-1.54871200	-0.79096100	-2.51383400
O	1.50826900	0.89271700	1.77119900
C	-0.91232800	-1.15286100	-3.72414000
H	-1.71776300	-1.38332600	-4.43014800
H	-0.30445800	-0.32467600	-4.12307200
H	-0.27641800	-2.04409100	-3.60084000
C	0.87427900	1.36316200	2.94374200
H	0.22960200	0.59096600	3.39404900
H	1.68079000	1.61162600	3.64235800
H	0.27518700	2.26701800	2.74746600
C	-2.89787800	0.22673500	-0.30383900
C	-3.90940300	-0.68293100	-0.50891800
S	-3.57016600	1.80791100	0.00098200

C	-5.22897500	-0.10193800	-0.44102300
O	-3.83846900	-2.01120000	-0.73637900
C	-5.22120700	1.24999400	-0.17294900
O	-6.26221500	-0.94082900	-0.63913300
C	-2.77596200	-2.75321800	-0.13639200
C	-6.29699100	2.23114200	-0.07376600
C	-7.57033300	-0.54598300	-0.22389900
C	-3.20292200	-4.21005300	-0.01763700
H	-2.56076500	-2.33494600	0.86067100
H	-1.86502300	-2.65937700	-0.74739900
C	-6.98678800	2.64562500	1.03802200
S	-6.84157200	3.14029200	-1.46929700
C	-8.47409200	-1.76894300	-0.27945000
H	-7.95062000	0.24062100	-0.89426000
H	-7.51482200	-0.12635100	0.79401300
C	-2.09047700	-4.99291200	0.68970300
H	-4.09103100	-4.22634700	0.63985000
C	-3.63732600	-4.80440900	-1.36625600
C	-7.94683300	3.67258700	0.76778300
O	-6.79670800	2.13032800	2.27743600
C	-7.99417600	4.05658000	-0.54606200
C	-9.92517500	-1.33006200	-0.05391000
H	-8.40153700	-2.15902000	-1.31107900
C	-7.99537800	-2.88823800	0.65824700
C	-2.42836300	-6.44634800	1.00241400
H	-1.16479800	-4.95439400	0.08860700
H	-1.85004700	-4.47619000	1.63554700
C	-2.54282500	-4.92567700	-2.42001100
H	-4.45285900	-4.17933800	-1.76168200
H	-4.08124700	-5.79651100	-1.18502500
O	-8.73871900	4.20294700	1.74043900
C	-7.84304800	2.48559000	3.18536900
C	-8.88238400	5.08661600	-1.15687600
C	-10.95948300	-2.43947800	-0.20780900
H	-10.02729600	-0.87121600	0.94567400
H	-10.16026800	-0.52653700	-0.77370000
C	-8.11843600	-2.60079900	2.15053000
H	-6.94280700	-3.09971600	0.41436700
H	-8.55017000	-3.80989000	0.41965500
H	-3.38464700	-6.48877900	1.55460800
H	-2.59394000	-7.00694800	0.06650300
C	-1.34665600	-7.15088100	1.81427700
H	-2.95080100	-5.34197000	-3.35318900
H	-2.10216600	-3.94783100	-2.66587900
H	-1.72520800	-5.58830900	-2.09728200
C	-8.21733000	3.94177600	3.04242600
H	-8.72288900	1.84736400	2.99873600
H	-7.45952000	2.28007800	4.19182600
H	-8.31849000	5.78820400	-1.78859300
H	-9.66748200	4.63424600	-1.78275700
H	-9.37441400	5.65989200	-0.36011400
H	-10.82202600	-2.93267200	-1.18709100
H	-10.79208400	-3.22250700	0.55150100
C	-12.39556400	-1.93951400	-0.09301000
H	-7.71484100	-3.43894500	2.73807600
H	-7.55994700	-1.69955300	2.44740900
H	-9.16486400	-2.45925100	2.46139300
C	-1.67616800	-8.60499300	2.12151100
H	-1.18485900	-6.60077400	2.75782400
H	-0.38957700	-7.09646700	1.26637000
H	-9.00855900	4.20573500	3.75415200
H	-7.33861200	4.58309900	3.22795900

C	-13.43127300	-3.04533200	-0.24090200
H	-12.57167800	-1.16292500	-0.85783200
H	-12.52739200	-1.43747500	0.88157800
H	-0.87936000	-9.08522500	2.70881800
H	-2.61141200	-8.68900300	2.69767700
H	-1.80621600	-9.18904400	1.19649900
H	-14.45602500	-2.65425600	-0.15504300
H	-13.34582300	-3.54354100	-1.21974900
H	-13.30370100	-3.81819200	0.53374200
C	2.85857500	-0.08709100	-0.45439200
C	3.85241500	0.81650900	-0.15292700
S	3.56137800	-1.62976900	-0.86828100
C	5.18109400	0.26243600	-0.24139300
O	3.74759100	2.11799000	0.18662800
C	5.20049900	-1.06177500	-0.62396500
O	6.19960100	1.09995400	0.02839400
C	2.73711800	2.91057000	-0.44037600
C	6.30155800	-1.97138100	-0.92345300
C	7.48136600	0.55820900	0.35030100
C	3.21758500	4.35477100	-0.48561000
H	1.80480200	2.84261000	0.13995200
H	2.53945200	2.51521700	-1.45061700
C	6.96743200	-2.82774500	-0.08240400
S	6.92044100	-2.15742100	-2.55242800
C	8.32075200	1.66220000	0.97706700
H	7.96524900	0.18200200	-0.56477500
H	7.35028600	-0.29191700	1.03932200
C	2.05603400	5.26309600	-0.90245000
H	3.48682200	4.61755900	0.55390000
C	4.48880500	4.51611100	-1.33366200
C	7.96611500	-3.61560400	-0.73887400
O	6.72040900	-2.92048000	1.24735000
C	8.06696200	-3.37626400	-2.08371500
C	9.76022900	1.16216000	1.14189900
H	8.33942200	2.49113700	0.24611900
C	7.68739500	2.21249100	2.26455100
C	2.36452300	6.75536300	-0.85352300
H	1.71406700	4.99357500	-1.91752200
H	1.19865000	5.05806000	-0.23760800
C	4.30819200	4.34192100	-2.83768300
H	5.22563400	3.78389400	-0.96879900
H	4.92437200	5.50859300	-1.13447500
O	8.73931600	-4.51511300	-0.06998000
C	7.74363100	-3.63371700	1.94743100
C	9.00141300	-4.02037100	-3.05053100
C	10.74737900	2.20990900	1.64391100
H	9.77865300	0.28912500	1.81836700
H	10.11109100	0.78670500	0.16465100
C	7.66375900	1.25659000	3.45218900
H	6.65769300	2.52031100	2.02550400
H	8.21758900	3.13467200	2.55205100
H	2.75290500	7.01443600	0.14812100
H	3.17332600	6.99900700	-1.56365200
C	1.15381200	7.62848900	-1.16535100
H	5.27701400	4.42174500	-3.35310900
H	3.88631700	3.35774400	-3.09436000
H	3.64569200	5.10795200	-3.26886300
C	8.16440800	-4.86872800	1.18689800
H	8.61081600	-2.97069000	2.10448900
H	7.31858400	-3.90330600	2.92154600
H	8.47649800	-4.37594000	-3.94901600
H	9.79319200	-3.32976200	-3.38045600

H	9.48358300	-4.88187600	-2.57001900
H	10.69074600	3.10385900	0.99679400
H	10.46000500	2.54881100	2.65398500
C	12.18640500	1.70676300	1.68282800
H	7.15821400	1.72300200	4.31091900
H	7.12199400	0.32534400	3.22516800
H	8.67647900	0.97863600	3.78210600
C	1.45951200	9.11913600	-1.12109100
H	0.34467700	7.39533200	-0.45118500
H	0.76153800	7.36098700	-2.16220700
H	8.93695400	-5.41520300	1.74081800
H	7.29846500	-5.53385900	1.02712700
C	13.17452300	2.74837100	2.18886500
H	12.48267300	1.37602400	0.67193400
H	12.23829600	0.80720600	2.32106300
H	0.56776900	9.72218200	-1.34820900
H	1.82226400	9.42259900	-0.12608300
H	2.23885200	9.38882400	-1.85156000
H	14.20267700	2.35709900	2.20426700
H	13.16936600	3.64627300	1.55059200
H	12.92553200	3.07098700	3.21237700
ii. Cation			
C	0.61508300	0.59835000	1.23038900
C	-0.76332700	0.75510400	1.26500500
C	-1.59375500	0.24876200	0.24544300
C	-0.99454200	-0.40314700	-0.85997400
C	0.39202700	-0.54725900	-0.89544300
C	1.21607300	-0.05567500	0.12409100
H	-1.23480600	1.23142300	2.12295300
H	0.86766600	-1.02729800	-1.74861300
O	-1.81898200	-0.80240800	-1.84582900
O	1.45128600	1.00342100	2.20945000
C	-1.25196000	-1.35424400	-3.02298300
H	-2.09720400	-1.58196500	-3.68057500
H	-0.58528100	-0.63169500	-3.51866500
H	-0.69791500	-2.28084800	-2.80938000
C	0.89677400	1.64307300	3.34411000
H	0.19831500	0.97918500	3.87814900
H	1.74307100	1.87914400	3.99766800
H	0.37893500	2.57563900	3.06889000
C	-3.02460600	0.48477600	0.29766300
C	-4.09823300	-0.35792100	-0.00590500
S	-3.55714800	2.07151000	0.80199000
C	-5.34619500	0.30731000	0.09106200
O	-4.03847300	-1.66955100	-0.29923200
C	-5.23230200	1.64902900	0.54660400
O	-6.56439000	-0.15009200	-0.15225100
C	-3.21396400	-2.49991000	0.54332400
C	-6.28150400	2.54762100	0.78884000
C	-6.80777400	-1.43119100	-0.78414700
C	-3.85273900	-3.87476500	0.67052900
H	-3.12898300	-2.02529600	1.53307200
H	-2.20698200	-2.56477500	0.10492800
C	-6.15845600	3.86543300	1.27527100
S	-7.98478700	2.16682800	0.56912000
C	-8.23890000	-1.43659200	-1.29327000
H	-6.65431200	-2.21512800	-0.03062200
H	-6.07786400	-1.57344900	-1.59076600
C	-3.06259500	-4.68806900	1.70348300
H	-4.86461400	-3.71280000	1.08364200
C	-4.02461400	-4.57514000	-0.68643100
C	-7.38941000	4.52479600	1.44902900

O	-4.97927100	4.42415900	1.54898600
C	-8.47745000	3.74413800	1.10689000
C	-8.62289700	-2.87739300	-1.65409900
H	-8.87340300	-1.12909100	-0.44276700
C	-8.46224600	-0.42031200	-2.42425600
C	-3.66296400	-6.04983200	2.03499500
H	-2.02150800	-4.82024700	1.36006700
H	-2.99549800	-4.09739700	2.63372700
C	-2.73750600	-5.02109400	-1.37030300
H	-4.57553800	-3.89470800	-1.35462800
H	-4.68176500	-5.44833200	-0.54684700
O	-7.48259500	5.79613400	1.89359600
C	-5.09563100	5.65807700	2.28674800
C	-9.90653600	4.13681700	1.17932600
C	-10.07554200	-3.05897100	-2.07986800
H	-7.95763100	-3.25588800	-2.45011500
H	-8.43040200	-3.51795600	-0.77607500
C	-7.77560300	-0.73865300	-3.74766600
H	-8.12857400	0.56720100	-2.06817500
H	-9.54614100	-0.32008700	-2.59323800
H	-4.72048400	-5.92090600	2.32828400
H	-3.67358600	-6.68936300	1.13593700
C	-2.91628900	-6.77616900	3.14877300
H	-2.95779300	-5.46213000	-2.35363900
H	-2.04563500	-4.18209100	-1.53874100
H	-2.19870500	-5.78141900	-0.78507100
C	-6.23860600	6.49139600	1.75814100
H	-5.24407800	5.41144500	3.34850900
H	-4.13917200	6.17594600	2.16034400
H	-10.45992600	3.80845600	0.28882800
H	-10.39301400	3.68309800	2.05761300
H	-9.98602900	5.22716400	1.27041900
H	-10.73825300	-2.63069300	-1.30639400
H	-10.27595500	-2.48694400	-3.00177900
C	-10.45027300	-4.51867000	-2.31316200
H	-7.95960000	0.06406200	-4.47680400
H	-6.68374600	-0.83245100	-3.64075000
H	-8.14605700	-1.67452600	-4.19235100
C	-3.50884400	-8.13869300	3.47983000
H	-2.91150300	-6.14462000	4.05436400
H	-1.85772600	-6.89392900	2.85796400
H	-6.33312800	7.41505600	2.33957600
H	-6.07617400	6.74509500	0.69827400
C	-11.89835300	-4.70515000	-2.74376900
H	-10.26152900	-5.09387800	-1.38990700
H	-9.77884000	-4.94700900	-3.07781000
H	-2.95074500	-8.63685600	4.28639300
H	-4.55724300	-8.04932500	3.80610800
H	-3.49264100	-8.80504800	2.60277900
H	-12.13890400	-5.76674000	-2.90279200
H	-12.59401700	-4.31620100	-1.98331200
H	-12.10711500	-4.17171000	-3.68469700
C	2.65800900	-0.29645900	0.08121100
C	3.74011700	0.52928800	0.30998000
S	3.20482800	-1.91823500	-0.26896800
C	5.00866500	-0.14747300	0.21618200
O	3.76356900	1.85350300	0.54615100
C	4.89125300	-1.49161300	-0.07859800
O	6.11066200	0.60338400	0.39480300
C	2.81536800	2.69315600	-0.12016500
C	5.87491300	-2.55408200	-0.18634400
C	7.32761300	0.21862800	-0.24860800

C	3.43724300	4.07036300	-0.30571700
H	1.90503700	2.77333900	0.49173500
H	2.54197300	2.23555400	-1.08526400
C	6.79366500	-2.98445900	0.74300100
S	5.92621300	-3.60200900	-1.58971700
C	8.25573800	1.42423500	-0.29875200
H	7.10237400	-0.13874400	-1.26659200
H	7.79205300	-0.60991600	0.30654900
C	2.35743400	5.05430800	-0.76864000
H	3.76943500	4.39104100	0.69857900
C	4.68560700	4.02647700	-1.20001600
C	7.52304300	-4.14238900	0.32592400
O	6.97815100	-2.39847100	1.95056200
C	7.16778100	-4.61066600	-0.91144600
C	9.55616300	1.00660700	-0.99641200
H	7.76560200	2.18106500	-0.93732000
C	8.45533100	2.06949500	1.08127700
C	2.81646000	6.50513200	-0.86266000
H	1.95231700	4.73509800	-1.74536400
H	1.50956300	4.99746100	-0.06347900
C	4.43338100	3.74411500	-2.67700100
H	5.35745500	3.25603700	-0.79109500
H	5.22562900	4.98188300	-1.10143600
O	8.47041800	-4.72395700	1.11044700
C	8.15025300	-2.87072700	2.62427200
C	7.73185400	-5.78733600	-1.63108800
C	10.53067600	2.14604000	-1.27286800
H	10.06539900	0.22614900	-0.40390900
H	9.29601500	0.52602200	-1.95605900
C	9.09929500	1.18325000	2.14087900
H	7.47141100	2.40478900	1.44366200
H	9.05524400	2.98476300	0.95411300
H	3.26634600	6.80814400	0.10007500
H	3.61830200	6.60105400	-1.61461800
C	1.68906800	7.46877000	-1.21732600
H	5.38597400	3.67798600	-3.22358700
H	3.90465800	2.79105800	-2.83435400
H	3.83734400	4.53569000	-3.15626200
C	8.30073000	-4.36602700	2.48145800
H	9.03741500	-2.36060900	2.21423500
H	8.03139500	-2.58963000	3.67732800
H	6.94026700	-6.43319300	-2.03752400
H	8.37818400	-5.48575400	-2.47017500
H	8.33830400	-6.38089100	-0.93442400
H	10.00578400	2.95228300	-1.81655000
H	10.87122600	2.59270100	-0.32312700
C	11.75045000	1.70822700	-2.07674600
H	9.21261000	1.73409900	3.08649100
H	8.48646700	0.29459100	2.35456900
H	10.10103000	0.83679800	1.84356800
C	2.14536300	8.91764900	-1.31701100
H	0.88817900	7.38409300	-0.46187700
H	1.23446700	7.15769800	-2.17430000
H	9.19823200	-4.71070000	3.00825500
H	7.41904600	-4.88435500	2.89525700
C	12.73008300	2.84136400	-2.34804500
H	11.41644600	1.27060800	-3.03381500
H	12.26650500	0.89452100	-1.53754700
H	1.31132200	9.58806600	-1.57254600
H	2.57415600	9.26736500	-0.36441500
H	2.91985000	9.03984100	-2.09080700
H	13.59739100	2.49570400	-2.92997100

	H	12.25135200	3.65538600	-2.91534100
	H	13.11016100	3.27409300	-1.40895700
e. EA (+1 charge)				
	C	1.68166100	-1.14595900	0.24508400
	C	0.45314000	-0.56668400	-0.16015900
	C	-0.66698900	-1.33633800	0.23994500
	C	-0.30039600	-2.42267100	1.01999200
	S	1.39682500	-2.55879700	1.25394500
	O	-1.89219300	-0.95982600	-0.12612500
	O	0.31896600	0.53738300	-0.90008900
	C	-2.98769900	-1.78888200	0.28665600
	C	-4.26970200	-1.22701500	-0.30539400
	H	-3.03837200	-1.79155800	1.38797900
	H	-2.80259800	-2.82118500	-0.05557100
	C	-5.45827300	-2.01165000	0.26296900
	H	-4.35299100	-0.18796700	0.06051900
	C	-6.82621100	-1.47587600	-0.14460300
	H	-5.38001900	-3.07414600	-0.02734300
	H	-5.38882800	-1.99863000	1.36472700
	H	-6.88260400	-0.39874300	0.09497500
	H	-6.95237000	-1.55058700	-1.23812000
	C	0.73085700	1.82302100	-0.34601600
	C	-0.46477500	2.73147200	-0.09934300
	H	1.38783600	2.27398500	-1.10057200
	H	1.32007900	1.64691000	0.56653200
	C	0.05408300	4.16671800	0.07099400
	H	-1.06361800	2.70399800	-1.02707100
	C	-1.03545200	5.22394100	0.21187500
	H	0.73153100	4.22152200	0.94146600
	H	0.67585800	4.41766500	-0.80591400
	H	-1.74686600	5.12860000	-0.62811900
	H	-1.62236900	5.04580200	1.12888700
	C	-7.97957700	-2.20489400	0.53641500
	C	-9.34781400	-1.67839700	0.12670400
	H	-7.86430200	-2.12365800	1.63142700
	H	-7.91358900	-3.28253900	0.30544800
	H	-10.15836800	-2.22169600	0.63460800
	H	-9.45535100	-0.61067300	0.37554300
	H	-9.50673600	-1.78124300	-0.95849000
	C	-0.48424100	6.64547300	0.24727300
	C	-1.56692200	7.70523600	0.39506600
	H	0.09452400	6.83348400	-0.67389300
	H	0.23606200	6.73392300	1.07936900
	H	-1.13967900	8.71872400	0.41590800
	H	-2.28345700	7.66285100	-0.44055600
	H	-2.13837400	7.56536300	1.32638100
	C	-4.22360500	-1.16262400	-1.84015500
	C	-4.20348200	-2.50564600	-2.56087400
	H	-3.33470300	-0.58001500	-2.12857000
	H	-5.08873000	-0.57641300	-2.18813500
	H	-4.14164900	-2.35534100	-3.64875700
	H	-3.33806600	-3.12170800	-2.27120500
	H	-5.11131500	-3.09574400	-2.36428000
	C	-1.36879300	2.25149900	1.04433700
	C	-0.75839600	2.30060100	2.44067100
	H	-1.69491300	1.22609300	0.81610000
	H	-2.28962500	2.85619200	1.03213400
	H	-1.46760700	1.90446900	3.18237700
	H	0.15922100	1.69687500	2.51990300
	H	-0.50546200	3.32673100	2.74744600
	C	2.97422300	-0.81436900	-0.18547200
	C	4.19349600	-1.35222200	0.29315100

S	3.30313000	0.29499400	-1.50940100
C	5.32389400	-0.87369500	-0.38663800
O	4.25030500	-2.21564500	1.29958600
C	5.01418200	0.02464900	-1.39768000
O	6.57596200	-1.26930500	-0.09603900
C	5.59190700	-2.43016700	1.79245000
C	6.57893400	-2.49293200	0.65195000
H	5.83288800	-1.60997200	2.48391000
H	5.56228500	-3.37731200	2.34042400
H	7.59590200	-2.61743000	1.03872700
H	6.34174000	-3.32895600	-0.02445900
C	5.97491300	0.70254500	-2.29758400
H	5.58873700	0.76966100	-3.32334500
H	6.16622600	1.73007800	-1.94737500
H	6.92810700	0.15978500	-2.29906900
H	-0.95581100	-3.14800900	1.49498000
f. EAB (+1 charge)			
C	3.95941300	-3.97691300	1.30069500
C	2.76474300	-3.26959200	1.25054600
C	2.40091500	-2.54998500	0.09369100
C	3.24110600	-2.58681400	-1.04691700
C	4.44370900	-3.30258400	-0.98341800
C	4.79627600	-3.98102400	0.17114600
H	2.10602600	-3.22303600	2.11645200
H	5.10935700	-3.34110200	-1.84329900
O	2.79719900	-1.94355000	-2.14076400
O	4.40912800	-4.66955100	2.36886300
C	3.59034200	-1.97281700	-3.31799300
H	3.03515800	-1.39364700	-4.06274000
H	4.57322700	-1.50662300	-3.15079200
H	3.72450100	-3.00349400	-3.68000100
C	3.59148400	-4.71145200	3.52410800
H	2.61403900	-5.17196500	3.30844700
H	4.12900500	-5.32801500	4.25224500
H	3.43734700	-3.70482400	3.94492700
C	1.11767100	-1.87314900	0.04126400
C	0.74056400	-0.61804500	-0.45206700
S	-0.26592100	-2.76320200	0.62835600
C	-0.66179400	-0.39949200	-0.39748700
O	1.51260300	0.37938400	-0.88972200
C	-1.37479200	-1.50930300	0.10715200
O	-1.14110100	0.78886500	-0.75046900
C	2.79569300	0.60164600	-0.27572600
C	-2.16753300	1.41281800	0.05526400
C	3.23911800	2.02043100	-0.59683400
H	3.52264800	-0.11296900	-0.68182200
H	2.70445400	0.43070600	0.80914200
C	-1.86974600	2.89940300	0.17830200
H	-2.17858200	0.93781800	1.04722800
H	-3.13781400	1.24122700	-0.42849100
C	4.71168900	2.18236400	-0.20155500
H	3.17948300	2.11409400	-1.69635100
C	2.30133300	3.08012000	-0.00093300
C	-2.91769900	3.52503500	1.10772500
H	-0.89031800	2.98429500	0.68049500
C	-1.73803900	3.58998900	-1.18755700
C	5.32907500	3.52106900	-0.59038400
H	4.82852100	2.02700900	0.88554300
H	5.29162800	1.37444700	-0.68082700
C	2.33200900	3.21401700	1.51735800
H	1.27795600	2.83951300	-0.32685200
H	2.53844700	4.05507200	-0.45565300

C	-2.67609200	4.99363000	1.43899700
H	-3.92488500	3.40904700	0.67021200
H	-2.93528400	2.95013700	2.05013400
C	-3.01450600	3.68178900	-2.01522800
H	-0.96808500	3.05531700	-1.76538800
H	-1.33688100	4.60294800	-1.02545500
H	5.16487600	3.69859800	-1.66857500
H	4.81355000	4.34368900	-0.06599000
C	6.82160100	3.60155500	-0.28812500
H	1.59505100	3.95923400	1.85222300
H	2.08748300	2.26780400	2.02483400
H	3.31590000	3.54179300	1.88543700
H	-1.64820200	5.11651100	1.82526000
H	-2.73034000	5.60328700	0.52105300
C	-3.66687600	5.54618500	2.45812300
H	-2.81172200	4.17348400	-2.97801100
H	-3.43340300	2.68984700	-2.24308400
H	-3.79810700	4.26578300	-1.50935200
C	7.44057900	4.93843600	-0.67129800
H	7.34388100	2.78621400	-0.81864500
H	6.98389300	3.41353400	0.78767700
C	-3.43419400	7.01429600	2.78624600
H	-3.60871100	4.94628400	3.38314700
H	-4.69356500	5.41098800	2.07512900
H	8.51637800	4.96596000	-0.44308300
H	7.32324300	5.13840700	-1.74824300
H	6.96350700	5.76971100	-0.12824800
H	-4.16179700	7.38349900	3.52408800
H	-2.42693100	7.17538300	3.20214900
H	-3.52349400	7.64361500	1.88655300
C	-2.76206100	-1.76777300	0.16714000
C	-3.76865400	-1.40438000	-0.74546300
S	-3.43314900	-2.82870400	1.39784700
C	-5.02208300	-1.98324700	-0.44659000
O	-3.54771600	-0.65655200	-1.82586600
C	-5.01330100	-2.78039800	0.68266300
O	-6.11149100	-1.80455900	-1.22235800
C	-4.75399000	-0.28421700	-2.52381700
C	-5.74307000	-1.42286800	-2.55249500
H	-5.18677800	0.59414800	-2.02210300
H	-4.44035100	-0.00797700	-3.53602000
H	-6.66500400	-1.10931300	-3.05396500
H	-5.32243900	-2.29500000	-3.07781100
C	-6.17065400	-3.49867000	1.26888700
H	-5.90072900	-4.52091000	1.56665500
H	-6.54118700	-2.97761200	2.16603100
H	-6.98573200	-3.53910600	0.53585700
H	5.73350100	-4.53596800	0.22063600

g. **EAB—EA (+1 charge)**

C	-2.73133400	-4.97176900	-0.91654000
C	-2.53034100	-3.59086700	-0.91464100
C	-3.05559600	-2.78082100	0.10474100
C	-3.77865100	-3.37966400	1.15503500
C	-3.99088200	-4.76237600	1.14030300
C	-3.47501700	-5.54903900	0.11633100
H	-1.97824000	-3.10525200	-1.71806900
H	-4.55761500	-5.24331300	1.93578600
O	-4.22595000	-2.55169800	2.13569000
O	-2.25825400	-5.82119800	-1.86538300
C	-5.04273400	-3.10659100	3.14814700
H	-5.31581700	-2.27376300	3.80558000
H	-5.95882500	-3.55269400	2.72858200

H	-4.50444800	-3.86894100	3.73421400
C	-1.52361100	-5.26804000	-2.93852500
H	-0.60976000	-4.76066700	-2.58801200
H	-1.24218900	-6.11058200	-3.58009900
H	-2.13019800	-4.55671500	-3.52270300
C	-2.80320900	-1.33149200	0.08773200
C	-3.65355400	-0.25247600	0.17670300
S	-1.15304300	-0.77935200	-0.05858400
C	-2.97784800	1.02105700	0.12201500
O	-4.99961900	-0.23393300	0.26320500
C	-1.60777600	0.91060200	0.00479700
O	-3.74901600	2.12529600	0.16123100
C	-5.74880200	-1.21758900	-0.45428900
C	-3.32583000	3.28936600	-0.55164800
C	-7.13518400	-0.65477500	-0.73508400
H	-5.83214500	-2.13274600	0.15058100
H	-5.21619100	-1.47272800	-1.38544500
C	-4.54067200	4.16751800	-0.81866400
H	-2.85465100	2.98245600	-1.49952900
H	-2.57279600	3.83296900	0.03889200
C	-8.04050100	-1.77489100	-1.25827000
H	-7.53632800	-0.33469500	0.24404500
C	-7.08336300	0.59350200	-1.62898200
C	-4.08553100	5.40952700	-1.59481600
H	-5.21237200	3.59222600	-1.48082900
C	-5.33432900	4.47397400	0.46076000
C	-9.50055800	-1.37840000	-1.44697700
H	-7.64186500	-2.16624600	-2.21113900
H	-7.99350900	-2.61985800	-0.54900400
C	-6.69847200	0.35169000	-3.08453100
H	-6.36567800	1.29386500	-1.17468100
H	-8.06287900	1.09700500	-1.59305200
C	-5.21574000	6.30329500	-2.09333000
H	-3.39296000	6.00674300	-0.97592900
H	-3.49212400	5.07675900	-2.46477100
C	-4.57935500	5.23949400	1.54113500
H	-5.68489500	3.51787900	0.87883600
H	-6.24393500	5.03033200	0.18377300
H	-9.88564100	-0.94749000	-0.50509800
H	-9.58185200	-0.57722900	-2.20150900
C	-10.38850400	-2.54474800	-1.86759500
H	-6.63713200	1.30566100	-3.62939500
H	-5.71667400	-0.13774600	-3.17942600
H	-7.43340100	-0.27707700	-3.60992300
H	-5.94003300	5.69275400	-2.66223400
H	-5.77564000	6.71999200	-1.23883300
C	-4.72722300	7.45166400	-2.97000000
H	-5.23176700	5.42976600	2.40631400
H	-3.71154600	4.67090400	1.90741300
H	-4.21607300	6.21581300	1.18519300
C	-11.84672700	-2.15210600	-2.05926700
H	-10.31732800	-3.34613200	-1.11139100
H	-9.99616800	-2.97864300	-2.80403400
C	-5.85137100	8.34942800	-3.46771300
H	-4.17383200	7.03946000	-3.83197000
H	-3.99590600	8.05422500	-2.40320700
H	-12.46127200	-3.01301000	-2.36182200
H	-12.27628600	-1.74661100	-1.12939100
H	-11.95299600	-1.37780600	-2.83564100
H	-5.46818000	9.16549800	-4.09822200
H	-6.58066300	7.78052800	-4.06605600
H	-6.39933800	8.80628000	-2.62833400

C	-0.55337400	1.90894100	-0.02616300
C	-0.26609400	2.90489400	0.87733900
S	0.65998400	1.90072300	-1.29115300
C	0.91755600	3.64237300	0.55444500
O	-1.00465200	3.15727800	1.98656800
C	1.54726500	3.21858900	-0.58546000
O	1.37233000	4.66251300	1.33265300
C	-0.65918500	4.39805800	2.61059000
C	0.83729000	4.59175800	2.65341100
H	-1.13157100	5.22899800	2.06093900
H	-1.07618700	4.35798400	3.62380200
H	1.08574300	5.54082500	3.14284200
H	1.31654300	3.76516600	3.20507400
C	2.79644500	3.76402400	-1.18822900
H	3.55211700	2.97902300	-1.34022500
H	2.61125100	4.24034800	-2.16330800
H	3.21954700	4.52204900	-0.51609500
H	-3.64223500	-6.62658300	0.10801100
C	2.81730700	-0.70933500	2.17706300
C	3.83854200	-0.47356400	1.21531400
C	4.56731100	0.72619000	1.47311100
C	4.10207900	1.36237700	2.60316500
S	2.78278800	0.56577200	3.37819800
O	5.55545300	1.12783200	0.65865200
O	3.97138500	-1.34642800	0.23493700
C	6.23670600	2.33414400	1.02710400
C	7.28998200	2.63948400	-0.02543100
H	6.68435000	2.19461200	2.02581800
H	5.50029700	3.15345000	1.08339900
C	8.37455300	1.55742700	-0.06642800
H	6.76352700	2.62596300	-0.99688600
C	9.37972800	1.71248000	-1.20183300
H	8.90874100	1.52954200	0.89968100
H	7.87940300	0.57751000	-0.16197200
H	8.83629200	1.81478900	-2.15874000
H	9.95166400	2.64789000	-1.07749000
C	5.09547500	-1.32787600	-0.68410000
C	4.91153000	-2.47291600	-1.66299000
H	6.01379100	-1.45276800	-0.09390300
H	5.12499500	-0.35189100	-1.18262000
C	6.20770700	-2.63224300	-2.46842500
H	4.78531000	-3.38750700	-1.05657700
C	6.22180600	-3.82688400	-3.41550200
H	6.41238600	-1.70939200	-3.03913000
H	7.04650100	-2.73592300	-1.75833100
H	5.95247300	-4.73976800	-2.85437900
H	5.44564900	-3.70630700	-4.19034900
C	10.35801600	0.54662300	-1.30244500
C	11.36874000	0.70685500	-2.42932200
H	9.79181800	-0.39083600	-1.44319200
H	10.89010900	0.43589100	-0.34135200
H	12.05818200	-0.14895800	-2.47871200
H	10.86692500	0.78761300	-3.40668200
H	11.97566900	1.61621800	-2.29476800
C	7.57134600	-4.03257700	-4.09499400
C	7.58961600	-5.22232500	-5.04436800
H	8.34995500	-4.16299000	-3.32319600
H	7.84334100	-3.11518400	-4.64576600
H	8.57505700	-5.34675900	-5.51710100
H	7.35349300	-6.15882100	-4.51451400
H	6.84674800	-5.10272400	-5.84890300
C	7.82581800	4.06831600	0.16502900

C	8.62839300	4.31852700	1.43756800
H	6.97088200	4.76469400	0.13054200
H	8.44548400	4.32368900	-0.70831400
H	8.96182300	5.36582700	1.47929000
H	8.03909000	4.12980500	2.34799800
H	9.52859800	3.68770800	1.48817200
C	3.64658000	-2.31363200	-2.52123800
C	3.65832200	-1.15677100	-3.51361900
H	2.78402500	-2.20362800	-1.84499300
H	3.47591600	-3.25685200	-3.06401000
H	2.69998800	-1.10473100	-4.05088300
H	3.80235700	-0.18378700	-3.01885600
H	4.45064100	-1.26516600	-4.26959600
C	1.94814900	-1.80558500	2.21213300
C	0.90913400	-2.02245600	3.14951100
S	2.01983400	-3.16237700	1.09603100
C	0.21774800	-3.22730900	2.95763600
O	0.63258400	-1.15960600	4.12173000
C	0.69860300	-3.96517100	1.88746400
O	-0.81647300	-3.61154300	3.73023100
C	-0.28409700	-1.68684600	5.10553800
C	-1.37174100	-2.50005000	4.44621500
H	0.29358300	-2.29710100	5.81495500
H	-0.70185000	-0.81723400	5.62314400
H	-2.03593600	-2.92285300	5.20772100
H	-1.96250000	-1.88494300	3.75008200
C	0.20264200	-5.28684300	1.43910100
H	0.39193600	-5.45451800	0.37187100
H	0.70385000	-6.09106600	2.00286200
H	-0.87595800	-5.36434900	1.63130300
H	4.46892400	2.29260500	3.02781600

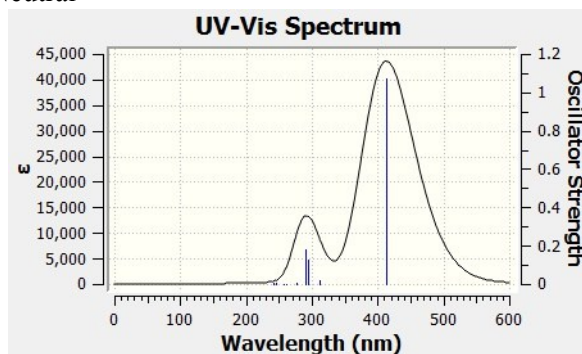
II. UV-Vis Spectra with keywords/settings: td=(nstates=10)/cc-pvdz
 scrf=(cpcm,solvent=dichloromethane) mpw1pbe *unless otherwise noted*

Table S1. Peak and Oscillator strengths (f) for all species

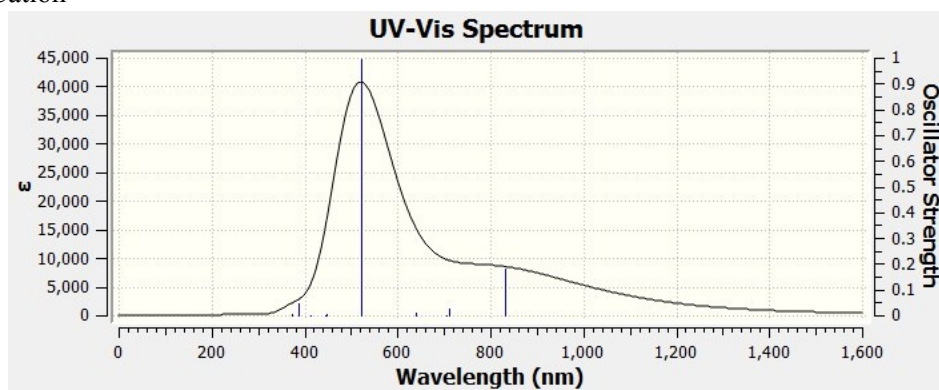
	EPE			EAE			EAAE			EABAE		EA	EAB	EA-- EAB
	0	1	2	0	1	2	0	1	2	0	1	1	1	1
□												430.5	1259	557.7
□	413.2	831.2	675.6	337.3	809.3	649.2	470.7	1074.3	699.8	337.2	1317			
f	1.07	0.18	0.2	0.84	0.20	0.23	0.64	0.44	1.59	0.95	0.34	0.16	0.18	0.06
□												398.6	664.8	
□	293.5	420.5	510.6	281.2	527.2	513.2	331	645.3	562.1	285.8	514.5			
f	0.13	1	1.12	0.14	0.92	1.09	0.17	0.52	0.21	0.11	0.40	0.42	0.13	
□													456.3	
□	290.3			253.2			305.8	600.1	386.6		473.5			
f	0.18			0.14			0.40	0.5	0.12		0.54		0.47	
□														
□				246.6			289.5							
f				0.18			0.16							
□														
□				244.7										
f				0.17										

III. EPE

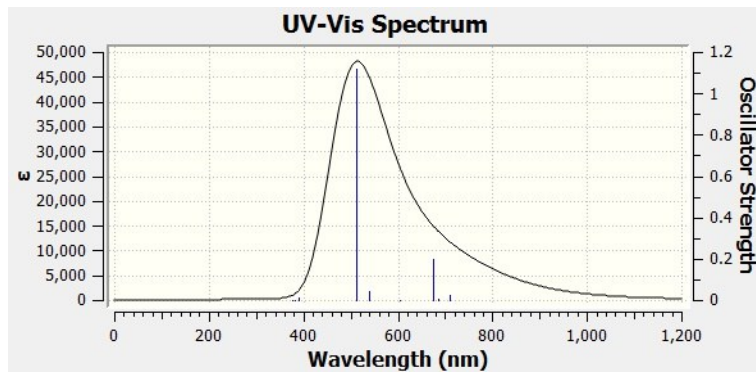
a. EPE - Neutral



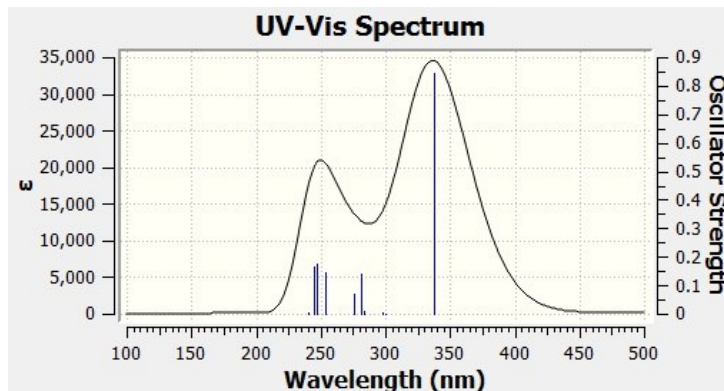
b. EPE - Cation



c. EPE - Dication



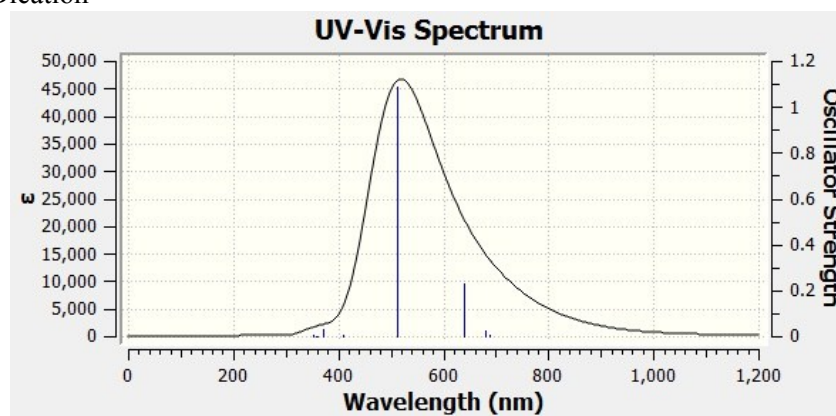
d. EAE - Neutral



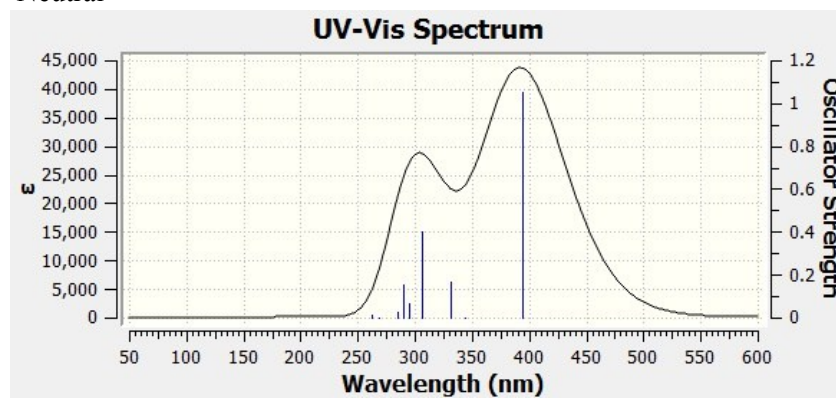
e. EAE -Cation



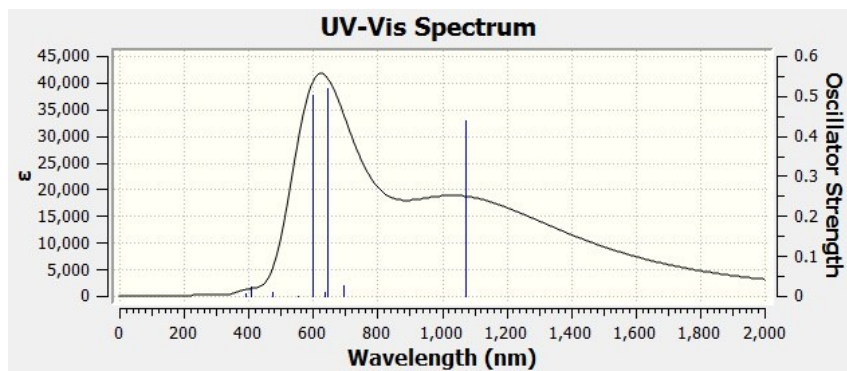
f. EAE -Dication



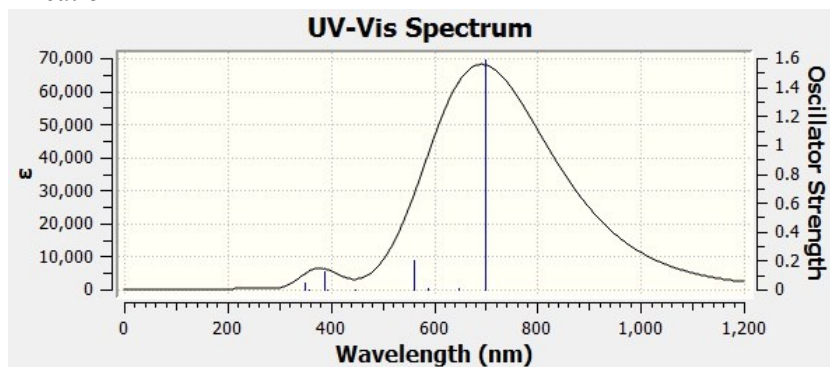
g. EAAE - Neutral



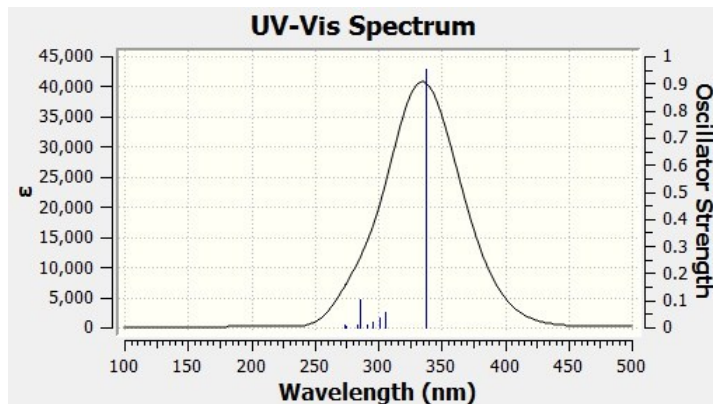
h. EAAE - Cation



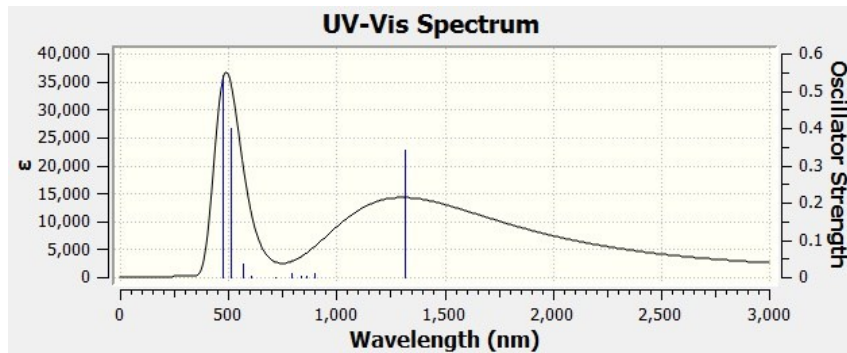
i. EAAE - Dication



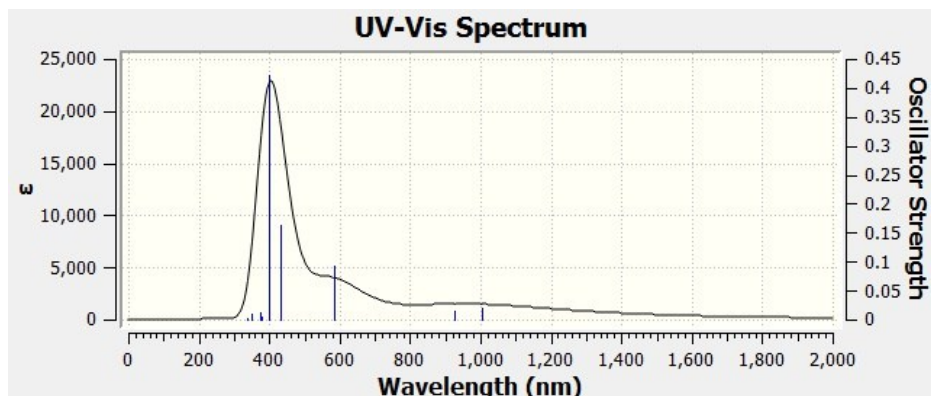
j. EABAE - Neutral



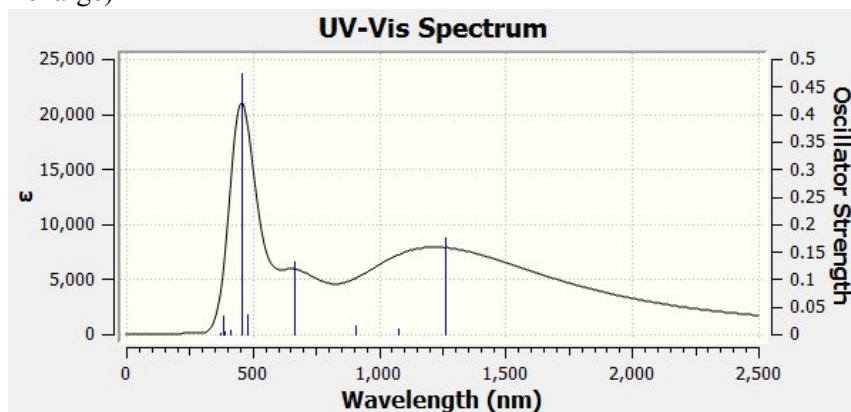
k. EABAE - Dication



l. EA (+1 charge)



m. EAB (+1 charge)



n. EAB—EA (+1 charge) with $nstates = 20$

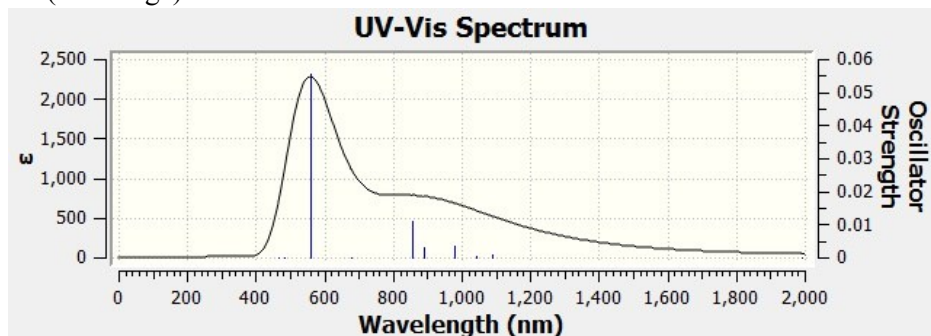


Figure S8. Calculated oscillator strengths of the compounds in various oxidation states

References

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- 2 J. A. Kerszulis, C. M. Amb, A. L. Dyer and J. R. Reynolds, *Macromolecules*, 2014, **47**, 5462–5469.
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