

## Supporting Information

### **Oxygen, sulfur and selenium terminated single-walled heterocyclic carbon nanobelts (SWHNBs) as potential 3D organic semiconductors**

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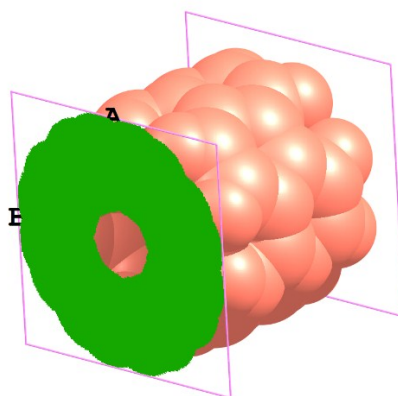
### Contents

	Page
1. Molecular Dimensions	S2
2. Ground State Geometries	S3
3. Optimised 1+ Cation Geometries	S7
4. Optimised 1- Anion Geometries	S11
5. Frontier Molecular Orbitals	S15
6. Vibrational Spectra	S16
7. Hole and Electron Reorganisation Energies, Transfer Integrals and Rates	S20
8. Hole and Electron Mobility Data	S21

## 1. Molecular Dimensions

<b>Table 1.</b> Molecular dimensions of the diameter, length, cross section and approximated volume.				
#	Diameter <sup>a</sup>	Length <sup>b</sup> / Å	Cross-section <sup>c</sup> / Å <sup>2</sup>	Volume <sup>d</sup> / Å <sup>3</sup>
1	5.618	6.567	44.06	289.3
2	7.059	6.588	58.46	385.1
3	8.379	6.597	72.92	481.1
4	5.667	6.683	44.83	308.6
5	6.992	6.58	60.18	396.0
6	8.194	4.398	75.76	333.2
7	5.627	8.315	45.49	378.2
8	6.97	8.303	60.28	500.5
9	8.226	8.27	76.84	635.5
10	45.631	8.952	48.43	433.5
11	6.977	8.963	62.58	560.9
12	8.243	8.947	78.08	698.6

<sup>a</sup>The largest diameter across the molecule (phenacene belt) plus twice the atomic radii of carbon; <sup>b</sup>distance between the centre of the peripheral atoms H, O, S and Se plus twice the atomic radius of those atoms; <sup>c</sup>the cross sectional area is taken around the widest diameter of each molecule; <sup>d</sup>the maximum VdW volume is approximated as the product of the molecular length and the nanobelt cross section area.



**Figure S1.** A typical volume calculation, using compound **3** as an example.



**Table 2. Continued**

4			5			6					
O	2.7419690000	-1.5497300000	0.0572950000	O	-2.6897870000	1.3150590000	-1.4948230000	O	-2.4990550000	-0.2632090000	2.6491000000
O	2.7417430000	0.8248000000	1.3129840000	O	-2.6897840000	-1.4948250000	-1.3150540000	O	-1.8666010000	-1.6802800000	-2.6491370000
O	2.7415550000	0.7254330000	-1.3705000000	O	2.6899210000	-0.1270970000	-1.9872780000	O	2.4990550000	0.2632090000	-2.6491010000
O	-2.7419690000	1.5497300000	-0.0572950000	O	2.6899270000	-1.9872780000	0.1270940000	O	1.0219650000	-2.2942490000	-2.6491750000
O	-2.7415550000	-0.7254330000	1.3705000000	O	-2.6897820000	-1.3150610000	1.4948300000	O	2.1762830000	-1.2566330000	2.6489520000
O	-2.7417430000	-0.8248000000	-1.3129840000	O	-2.6897850000	1.4948290000	1.3150660000	O	-0.5223640000	-2.4574200000	-2.6486710000
C	-1.8476390000	1.4539530000	1.0188370000	O	2.6899310000	0.1270990000	1.9872770000	O	-2.1762830000	1.2566330000	-2.6489520000
C	-1.8472350000	0.2854020000	1.7516090000	O	2.6899280000	1.9872840000	-0.1271020000	O	0.5223640000	2.4574200000	-2.6486710000
C	-0.5872180000	-0.3021510000	2.1448150000	C	-1.8343980000	2.1932110000	-0.8307390000	O	-1.0219640000	2.2942490000	2.6491750000
C	-0.5877670000	2.0643210000	0.6604250000	C	-0.5987110000	2.3243900000	-1.5535140000	O	1.8666020000	1.6802800000	2.6491380000
C	-1.8473960000	-1.6606920000	-0.6286070000	C	-0.5987560000	1.2447080000	-2.5032750000	C	-2.5696950000	-1.3855720000	-2.6491560000
C	-1.8472110000	-1.6095130000	0.7497700000	C	-1.8344750000	0.5442700000	-2.2813080000	C	-2.8013190000	0.8202140000	1.8274140000
C	-0.5871730000	-1.6040770000	1.4569320000	C	-1.8343980000	-0.8307430000	-2.1932090000	C	-3.2488960000	-1.0555690000	0.6062770000
C	-1.8474930000	0.1551750000	-1.7679080000	C	-0.5987110000	-1.5535150000	-2.3243880000	C	-3.3970000000	0.3561830000	0.6065330000
C	-1.8476470000	1.3745390000	-1.1232860000	C	-0.5987530000	-2.5032780000	-1.2447090000	C	-2.0076860000	-2.7629550000	-0.6070080000
C	-0.5877930000	2.0097340000	-0.8110920000	C	-1.8344700000	-2.2813100000	-0.5442680000	C	-2.9574730000	-1.7079930000	-2.6068440000
C	-0.5873260000	-1.7073940000	-1.3342950000	C	0.5986840000	-0.8900060000	-2.6503310000	C	-1.2641260000	-2.6303080000	-1.8276590000
C	-0.5874170000	-0.4600250000	-2.1165390000	C	0.5986870000	0.5451040000	-2.7420280000	C	-2.7483860000	-0.9820880000	-1.8274800000
C	0.5877930000	-2.0097340000	0.8110920000	C	1.8343380000	0.9634600000	-2.1378750000	C	2.5696940000	1.3855720000	-1.8271560000
C	1.8476470000	-1.3745390000	1.1232870000	C	1.8344130000	-1.2280230000	-1.9979930000	C	3.2488950000	1.0555680000	-0.6062770000
C	0.5877670000	-2.0643210000	-0.6604250000	C	1.8343420000	-2.1378780000	-0.9634650000	C	3.3970000000	-1.3561830000	-0.6065330000
C	1.8474930000	-0.1551750000	1.7679080000	C	0.5986910000	-2.7420280000	-0.5451060000	C	2.8013200000	-0.8202140000	-1.8274150000
C	0.5874170000	0.4600250000	2.1165390000	C	0.5986900000	-2.6503310000	0.8900050000	C	2.1110880000	-2.0146150000	-1.8272810000
C	1.8476390000	-1.4539530000	-1.0188370000	C	1.8344190000	-1.9979890000	1.2280190000	C	2.0073280000	-2.7628770000	-0.6068230000
C	1.8472350000	-0.2854020000	-1.7516090000	C	-1.8343950000	-2.1932160000	0.8307460000	C	0.7106840000	-3.3405550000	-0.6069150000
C	0.5873260000	1.7073940000	1.3342950000	C	-0.5987050000	-2.3243900000	1.5535150000	C	0.0852650000	-2.9172320000	-1.8276540000
C	1.8473960000	1.6606920000	0.6286070000	C	-0.5987480000	-1.2447090000	2.5032770000	C	2.5386100000	-2.2848420000	0.6061570000
C	0.5872180000	0.3021510000	-2.1448150000	C	-1.8344670000	-0.5442710000	2.2813090000	C	3.2486680000	-1.0556320000	0.6062620000
C	1.8472110000	1.6095130000	-0.7497700000	C	-1.8343940000	0.8307420000	2.1932160000	C	2.8935640000	-0.3899160000	1.8274830000
C	0.5871730000	1.6040770000	-1.4569320000	C	-0.5987050000	1.5535130000	2.3243890000	C	1.7837650000	-2.3102960000	1.8268940000
				C	-0.5987510000	2.5032760000	1.2447090000	C	0.5234840000	-2.8715650000	1.8270080000
				C	-1.8344720000	2.2813090000	0.5442730000	C	-0.0001950000	-3.4154570000	0.6060030000
				C	0.5986910000	0.8900060000	2.6503280000	C	-1.3886840000	-3.1202400000	0.6059700000
				C	0.5986950000	-0.5451040000	2.7420240000	C	-1.6460540000	-2.4103030000	1.8267950000
				C	1.8343470000	-0.9634610000	2.1378730000	C	-2.8935640000	0.3899160000	-1.8274830000
				C	1.8344200000	1.2280230000	1.9979870000	C	-3.2486680000	1.0556320000	-0.6062620000
				C	1.8343440000	2.1378750000	0.9634570000	C	-2.5386110000	2.2848420000	-0.6061570000
				C	0.5986900000	2.7420270000	0.5451030000	C	-1.7837660000	2.3102970000	-1.8268940000
				C	0.5986850000	2.6503300000	-0.8900080000	C	-0.5234840000	2.8715650000	-1.8270080000
				C	1.8344150000	1.9979950000	-1.2280280000	C	0.0001950000	3.4154560000	-0.6060030000
								C	1.3886850000	3.1202400000	-0.6059700000
								C	1.6460540000	2.4103030000	-1.8267960000
								C	-0.7106840000	3.3405550000	0.6069160000
								C	-2.0073280000	2.7628770000	0.6068230000
								C	-2.1110880000	2.0146150000	1.8272800000
								C	-0.0852650000	2.9172310000	1.8276540000
								C	1.2641260000	2.6303090000	1.8276590000
								C	2.0076860000	2.7629550000	0.6070080000
								C	2.9574730000	1.7079930000	0.6068440000
								C	2.7483850000	0.9820880000	1.8274800000

**Table 2. Continued.**

7			8			9					
S	3.1574500000	-1.1915250000	-1.5123230000	S	-3.1515240000	0.7397750000	2.2797100000	S	3.1151960000	2.7266290000	-1.1475950000
S	3.1574470000	1.9056260000	-0.2755920000	S	-3.1515800000	2.2797720000	-0.7396940000	S	3.1206350000	1.9494300000	2.2161720000
S	3.1572090000	-0.7141910000	1.7878970000	S	3.1515200000	2.1350980000	1.0889860000	S	-3.1551690000	2.8413770000	0.6607130000
S	-3.1575170000	-1.9052960000	0.2758030000	S	3.1514280000	1.0890220000	-2.1351750000	S	-3.1363750000	0.2335740000	2.9245230000
S	-3.1573290000	1.1916240000	1.5120950000	S	-3.1516360000	-0.7397700000	-2.2797750000	S	3.1551760000	-2.8414510000	-0.6607400000
S	-3.1571330000	0.7139180000	-1.7877960000	S	-3.1515790000	-2.2797360000	0.7398580000	S	3.1363890000	-0.2335610000	-2.9246760000
C	-0.5911210000	-1.8882860000	1.0182340000	S	3.1514300000	-2.1351400000	-1.0890990000	S	-3.1206330000	-1.9493710000	-2.2161250000
C	-1.8680930000	-1.3016810000	1.3982360000	S	3.1515230000	-1.0890540000	2.1350560000	S	-3.1451400000	1.4901930000	-2.5173470000
C	-0.5911470000	-2.0991080000	-0.4410980000	C	-1.8636810000	-0.4960940000	2.4923360000	S	-3.1151840000	-2.7265210000	1.1475280000
C	-1.8677240000	-0.0196440000	1.9096500000	C	-0.6001250000	0.1430270000	2.7813860000	S	3.1452320000	-1.4903840000	2.5176550000
C	-0.5909260000	0.6673230000	2.0377840000	C	-0.6001360000	1.5171800000	2.3358110000	C	1.8458680000	2.1999290000	-2.2962830000
C	-1.8679170000	-1.6449540000	-0.9724260000	C	-1.8637220000	1.8651460000	1.7267340000	C	0.5855240000	2.8134490000	-1.9690690000
C	-1.8679070000	-0.5603760000	-1.8267230000	C	-1.8637000000	2.4923530000	0.4961370000	C	0.5814840000	3.3730500000	-0.6527490000
C	-0.5908860000	1.8257740000	1.1260650000	C	-1.8637970000	1.7266950000	-1.8650280000	C	1.8388050000	3.1847940000	0.0223600000
C	-1.8679700000	1.8624410000	0.4281760000	C	-0.6002130000	2.3358160000	-1.5171240000	C	1.8409310000	2.8736250000	1.3695880000
C	-0.5909420000	0.0624640000	-2.1436710000	C	-0.6001570000	2.7814120000	-0.1429980000	C	1.8545350000	0.9718900000	3.0217860000
C	-1.8677970000	1.6645040000	-0.9379390000	C	1.8638370000	1.4116100000	2.1132260000	C	0.5935140000	1.6659210000	3.0006300000
C	-0.5909930000	1.4315620000	-1.5970010000	C	0.6002610000	2.0677030000	1.8655200000	C	0.5858810000	2.7458040000	2.0627280000
C	0.5907340000	-1.8254740000	-1.1260710000	C	0.6003090000	2.7239790000	0.5785040000	C	-1.8839940000	3.1065300000	-0.5730100000
C	0.5908660000	-0.6673620000	-2.0375920000	C	1.8639310000	2.5395120000	-0.0981730000	C	-0.6303710000	3.4268440000	0.0577410000
C	0.5907960000	-1.4314060000	1.5968800000	C	1.8637660000	2.1132590000	-1.4116530000	C	-0.6280920000	3.1049280000	1.4515280000
C	1.8679890000	-1.6643670000	0.9379210000	C	0.6001680000	1.8655180000	-2.0676890000	C	-1.8799320000	2.5394690000	1.8817690000
C	1.8678280000	-1.8623560000	-0.4279450000	C	0.6002150000	0.5785000000	-2.7239530000	C	-1.8725850000	1.4953870000	2.7886030000
C	0.5909950000	1.8881500000	-1.0179390000	C	1.8638460000	-0.0981830000	-2.5395060000	C	-0.6131310000	1.0006600000	3.2794440000
C	1.8680260000	1.3016050000	-1.3983260000	C	-1.8637710000	0.4960870000	-2.4922110000	C	-0.6029080000	-0.4242440000	3.4043850000
C	1.8679530000	0.0195580000	-1.9093960000	C	-0.6002420000	-0.1430110000	-2.7814070000	C	-1.8544750000	-1.0145060000	3.0081060000
C	0.5908790000	-0.0625410000	2.1435500000	C	-0.6002530000	-1.5171580000	-2.3358330000	C	1.8840530000	-3.1063680000	0.5730220000
C	0.5909820000	2.0987980000	0.4408100000	C	-1.8638230000	-1.8650830000	-1.7266870000	C	0.6302990000	-3.4267290000	-0.0578030000
C	1.8681100000	1.6447070000	0.9721220000	C	-1.8637520000	-2.4922080000	-0.4960410000	C	0.6280380000	-3.1048200000	-1.4514710000
C	1.8679260000	0.5602530000	1.8264730000	C	-1.8637450000	-1.7267350000	1.8652000000	C	1.8799830000	-2.5393730000	-1.8817690000
				C	-0.6001720000	-2.3358350000	1.5171920000	C	1.8726220000	-1.4953720000	-2.7885600000
				C	-0.6002060000	-2.7813910000	0.1430390000	C	1.8544750000	1.0145210000	-3.0080580000
				C	1.8637220000	-1.4116650000	-2.1132810000	C	0.6028500000	0.4241800000	-3.4043410000
				C	0.6001440000	-2.0677240000	-1.8655550000	C	0.6130770000	-1.0006140000	-3.2794630000
				C	0.6002250000	-2.7239370000	-0.5785120000	C	-1.8408780000	-2.8736600000	-1.3696630000
				C	1.8638760000	-2.5394720000	0.0981370000	C	-0.5859330000	-2.7458850000	-2.0627730000
				C	1.8637960000	-2.1132440000	1.4116160000	C	-0.5935840000	-1.6659160000	-3.0007370000
				C	0.6002390000	-1.8655570000	2.0677340000	C	-1.8544760000	-0.9719720000	-3.0219410000
				C	0.6003170000	-0.5785150000	2.7239570000	C	-1.8643620000	0.4055240000	-3.1427040000
				C	1.8639590000	0.0981300000	2.5394780000	C	-0.6135970000	1.1106030000	-3.2440970000
								C	-0.6224870000	2.3367670000	-2.5075320000
								C	-1.8800610000	2.5655680000	-1.8457620000
								C	-1.8458680000	-2.1999810000	2.2962960000
								C	-1.8387660000	-3.1848340000	-0.0223460000
								C	-0.5855800000	-2.8134560000	1.9691500000
								C	-0.5815350000	-3.3730600000	0.6527050000
								C	0.6135230000	-1.1106500000	3.2440760000
								C	0.6224100000	-2.3367210000	2.5075650000
								C	1.8643500000	-0.4054770000	3.1426820000
								C	1.8800540000	-2.5655560000	1.8457090000

**Table 2. Continued.**

10			11			12					
Se	3.2761110000	-1.6806750000	1.1638280000	Se	-3.2815840000	-0.3924010000	-2.5198210000	Se	3.2722190000	3.0654690000	0.3960300000
Se	3.2764090000	1.8485120000	0.8730500000	Se	-3.2815840000	-2.5198900000	0.3924060000	Se	-3.2739280000	2.2447100000	2.1221600000
Se	3.2760550000	-0.1679310000	-2.0368450000	Se	3.2815920000	-2.0582000000	-1.5042610000	Se	-3.2722190000	-3.0654710000	-0.3960310000
Se	-3.2761110000	1.6806730000	-1.1638260000	Se	3.2815830000	-1.5042400000	2.0581970000	Se	-3.2723920000	-1.3244280000	2.7903020000
Se	-3.2760550000	0.1679320000	2.0368470000	Se	-3.2815950000	0.3924000000	2.5198160000	Se	3.2744540000	-2.7120900000	1.4805130000
C	-3.2764090000	-1.8485130000	-0.8730510000	Se	-3.2815970000	2.5198420000	-0.3924070000	Se	3.2733760000	0.5708830000	3.0345110000
C	-1.8617770000	1.9339070000	0.1549350000	Se	3.2815720000	2.0581790000	1.5042340000	Se	-3.2744530000	2.7120880000	-1.4805110000
C	-1.8615670000	1.3476310000	1.3945150000	Se	3.2815790000	1.5042440000	-2.0581590000	Se	-3.2733760000	-0.5708820000	-3.0345110000
C	-0.5907960000	0.9019420000	1.9477490000	C	-1.8594650000	0.9130940000	-2.4119380000	Se	3.2723920000	1.3244280000	-2.7903010000
C	-0.5908030000	2.0785370000	-0.5404370000	C	-0.6000050000	0.3025410000	-2.7715910000	Se	3.2739280000	-2.2447100000	-2.1221610000
C	-1.8614910000	-1.8819130000	0.4693210000	C	-0.6000020000	-1.1300390000	-2.5484490000	C	1.8563440000	2.7606540000	1.6625630000
C	-1.8615800000	-1.1011550000	1.5966360000	C	-1.8593290000	-1.6024890000	-2.0195240000	C	1.8559140000	3.0926220000	-0.9058660000
C	-0.5906520000	-0.5708740000	2.0691370000	C	-1.8594580000	-2.4119510000	-0.9130870000	C	0.6042110000	3.2447230000	1.1438440000
C	-1.8615060000	-0.8324030000	-1.7508900000	C	-0.5999950000	-2.7716220000	-0.3025400000	C	0.6040780000	3.4287490000	-0.2803900000
C	-1.8614890000	0.5342510000	-1.8630160000	C	-0.5999970000	-2.5484620000	1.1300530000	C	-0.6056330000	1.9518920000	2.8318950000
C	-0.5907500000	1.2361330000	-1.7544450000	C	-1.8593300000	-2.0195470000	1.6024910000	C	-0.6062700000	2.9381170000	1.7880160000
C	-0.5907450000	-2.1383660000	-0.1931130000	C	0.6000800000	-2.6016470000	-1.0033100000	C	-1.8570770000	1.2544330000	2.9668590000
C	-0.5908020000	-1.5070940000	-1.5291480000	C	0.6001580000	-1.7461340000	-2.1738730000	C	-1.8581960000	3.0323790000	1.0844140000
C	0.5907480000	-1.2361330000	1.7544450000	C	1.8593240000	-1.0591050000	-2.3502780000	C	-1.8563440000	-2.7606540000	-1.6625640000
C	1.8614900000	-0.5342530000	1.8630180000	C	1.8593310000	-2.5611650000	-0.2956140000	C	-0.6042110000	-3.2447230000	-1.1438450000
C	0.5908020000	-2.0785370000	0.5404370000	C	1.8593290000	-2.3502330000	1.0590990000	C	-0.6040780000	-3.4287480000	-0.2803900000
C	1.8615060000	0.8324010000	1.7508840000	C	0.6001540000	-2.1738490000	1.7461300000	C	-1.8559140000	-3.0926200000	0.9058660000
C	0.5908030000	1.5070950000	1.5291470000	C	0.6000700000	-1.0032970000	2.6016520000	C	-1.8560460000	-2.4346410000	2.1103350000
C	1.8617780000	-1.9339080000	-0.1549340000	C	1.8593130000	-0.2956020000	2.5612080000	C	-0.6042880000	-2.0903180000	2.7313710000
C	1.8615670000	-1.3476260000	-1.3945110000	C	-1.8594690000	-0.9130750000	2.4119070000	C	-0.6045670000	-0.7926420000	3.3466370000
C	0.5907450000	2.1383670000	0.1931110000	C	-0.6000140000	-0.3025210000	2.7715890000	C	-1.8565690000	-0.0945730000	3.2197140000
C	1.8614900000	1.8819170000	-0.4693240000	C	-0.6000150000	1.1300600000	2.5484520000	C	0.6063840000	-2.6085040000	2.2415960000
C	0.5907970000	-0.9019400000	-1.9477480000	C	-1.8593420000	1.6025150000	2.0195420000	C	0.6065290000	-3.2965630000	0.9811080000
C	1.8615790000	1.1011590000	-1.5966390000	C	-1.8594720000	2.4119520000	0.9130800000	C	1.8583740000	-3.2089730000	0.2766540000
C	0.5906520000	0.5708750000	-2.0691380000	C	-0.6000180000	2.7716280000	0.3025320000	C	1.8579910000	-1.9684160000	2.5493510000
				C	-0.6000140000	2.5484830000	-1.1300550000	C	1.8577820000	-0.7280130000	3.1370640000
				C	-1.8593340000	2.0195590000	-1.6025050000	C	0.6059060000	-0.0851200000	3.4380960000
				C	0.6000670000	2.6016660000	1.0033060000	C	0.6052980000	1.3263550000	3.1730580000
				C	0.6001470000	1.7461440000	2.1738520000	C	1.8568590000	1.8177750000	2.6599520000
				C	1.8593090000	1.0591150000	2.3502550000	C	-1.8583740000	3.2089740000	-0.2766550000
				C	1.8593120000	2.5612180000	0.2956140000	C	-0.6065300000	3.2965640000	-0.9811080000
				C	1.8593160000	2.3503070000	-1.0591100000	C	-0.6063850000	2.6085050000	-2.2415950000
				C	0.6001520000	2.1738900000	-1.7461370000	C	-1.8579900000	1.9684160000	-2.5493500000
				C	0.6000770000	1.0033160000	-2.6016190000	C	-1.8577820000	0.7280130000	-3.1370630000
				C	1.8593190000	0.2956220000	-2.5611530000	C	-0.6059060000	0.0851210000	-3.4380970000
								C	-0.6052970000	-1.3263540000	-3.1730580000
								C	-1.8568590000	-1.8177760000	-2.6599540000
								C	0.6045670000	0.7926420000	-3.3466370000
								C	0.6042880000	2.0903190000	-2.7313720000
								C	1.8560450000	2.4346410000	-2.1103340000
								C	1.8565690000	0.0945740000	-3.2197160000
								C	1.8570760000	-1.2544310000	-2.9668570000
								C	0.6056330000	-1.9518920000	-2.8318960000
								C	0.6062700000	-2.9381160000	-1.7880160000
								C	1.8581970000	-3.0323790000	-1.0844140000



**Table 3. Continued.**

4			5			6					
O	2.7419690000	-1.5497300000	0.0572950000	O	2.6570130000	-1.7951640000	-0.7577230000	O	1.8426040000	1.6591680000	2.6197000000
O	2.7417430000	0.8248000000	1.3129840000	O	2.6569890000	0.7577660000	-1.7951580000	O	-1.0092780000	2.2661550000	2.6201690000
O	2.7415550000	0.7254330000	-1.3705000000	O	-2.6568690000	-0.7334740000	-1.8052230000	O	0.5153480000	2.4267960000	-2.6190660000
O	-2.7419690000	1.5497300000	-0.0572950000	O	-2.6569010000	1.8051710000	-0.7334710000	O	-2.1473100000	1.2404570000	-2.6191960000
O	-2.7415550000	-0.7254330000	1.3705000000	O	2.6569490000	1.7951990000	0.7577580000	O	-0.5153480000	-2.4267960000	2.6190660000
O	-2.7417430000	-0.8248000000	-1.3129840000	O	2.6569720000	-0.7577150000	1.7952030000	O	2.1473100000	-1.2404570000	2.6191960000
C	-1.8476390000	1.4539530000	1.0188370000	O	-2.6569120000	0.7334230000	1.8051730000	O	1.0092780000	-2.2661550000	-2.6201690000
C	-1.8472350000	0.2854020000	1.7516090000	O	-2.6568800000	-1.8052230000	0.7334260000	O	2.4659530000	0.2594240000	-2.6193170000
C	-0.5872180000	-0.3021510000	2.1448150000	C	1.8285080000	-2.3469220000	0.2016750000	O	-1.8426040000	-1.6591680000	-2.6197000000
C	-0.5877670000	2.0643210000	0.6604250000	C	0.6006170000	-2.7735170000	-0.3896200000	O	-2.4659530000	-0.2594240000	2.6193170000
C	-1.8473960000	-1.6606920000	-0.6286070000	C	0.6006150000	-2.2138560000	-1.7153540000	C	2.7514070000	0.9883870000	1.8205640000
C	-1.8472110000	-1.6095130000	0.7497700000	C	1.8282110000	-1.4921310000	-1.8218100000	C	2.9626650000	1.7119740000	0.6079760000
C	-0.5871730000	-1.6040770000	1.4569320000	C	1.8285030000	-0.2016380000	-2.3469070000	C	2.0119200000	2.7677720000	0.6081630000
C	-1.8474930000	0.1551750000	-1.7679080000	C	1.8281760000	1.8218550000	-1.4921390000	C	1.2704110000	2.6330310000	1.8207220000
C	-1.8476470000	1.3745390000	-1.1232860000	C	0.6005810000	1.7153670000	-2.2138570000	C	-0.0902580000	2.9225340000	1.8208900000
C	-0.5877930000	2.0097340000	-0.8110920000	C	0.6006070000	0.3896330000	-2.7735140000	C	-2.1124870000	2.0229640000	1.8211390000
C	-0.5873260000	-1.7073940000	-1.3342950000	C	-1.8284140000	-1.8022430000	-1.5168120000	C	-2.0112050000	2.7695810000	0.6081670000
C	-0.5874170000	-0.4600250000	-2.1165390000	C	-0.6005830000	-1.6856210000	-2.2367310000	C	-0.7131620000	3.3471900000	0.6083070000
C	0.5877930000	-2.0097340000	0.8110920000	C	-0.6005750000	-0.3524920000	-2.7786520000	C	1.6445650000	2.4174210000	-1.8198650000
C	1.8476470000	-1.3745390000	1.1232870000	C	-1.8282580000	0.2329970000	-2.3438270000	C	1.3902890000	3.1266460000	-0.6070910000
C	0.5877670000	-2.0643210000	-0.6604250000	C	-1.8284420000	1.5167780000	-1.8022390000	C	0.0006780000	3.4228720000	-1.82070810000
C	1.8474930000	-0.1551750000	1.7679080000	C	-0.6006270000	2.2367280000	-1.6856240000	C	-0.5200190000	2.8789590000	-1.8202360000
C	0.5874170000	0.4600250000	2.1165390000	C	-0.6006280000	2.7786460000	-0.3524940000	C	-1.7906330000	2.3122240000	-1.8201280000
C	1.8476390000	-1.4539530000	-1.0188370000	C	-1.8282990000	2.3437950000	0.2329990000	C	-2.5439260000	2.2890680000	-0.6074000000
C	1.8472350000	-0.2854020000	-1.7516090000	C	1.8284570000	2.3469460000	-0.2016410000	C	-3.2541520000	1.0585410000	-0.6077060000
C	0.5873260000	1.7073940000	1.3342950000	C	0.6005560000	2.7735310000	0.3896320000	C	-2.8967970000	0.3951460000	-1.8204510000
C	1.8473960000	1.6606920000	0.6286070000	C	0.6005400000	2.2138700000	1.7153640000	C	-1.6445650000	-2.4174210000	1.8198650000
C	0.5872180000	0.3021510000	-2.1448150000	C	1.8281420000	1.4921630000	1.8218420000	C	-1.3902890000	-3.1266460000	0.6070910000
C	1.8472110000	1.6095130000	-0.7497700000	C	1.8284610000	0.2016770000	2.3469580000	C	-0.0006780000	-3.4228720000	0.6070810000
C	0.5871730000	1.6040770000	-1.4569320000	C	1.8281760000	-1.8217980000	1.4921540000	C	0.5200190000	-2.8789590000	1.8202360000
				C	0.6005740000	-1.7153530000	2.2138700000	C	1.7906330000	-2.3122240000	1.8201280000
				C	0.6005660000	-0.3896200000	2.7735330000	C	2.8967970000	-0.3951460000	1.8204510000
				C	-1.8284740000	1.8022020000	1.5167770000	C	3.2541520000	-1.0585410000	0.6077060000
				C	-0.6006550000	1.6856090000	2.2367250000	C	2.5439260000	-2.2890680000	0.6074000000
				C	-0.6006330000	0.3524820000	2.7786510000	C	0.0902580000	-2.9225340000	-1.8208900000
				C	-1.8282940000	-0.2330340000	2.3438010000	C	0.7131620000	-3.3471900000	-0.6083070000
				C	-1.8284460000	-1.5168120000	1.8022060000	C	2.0112050000	-2.7695810000	-0.6081670000
				C	-0.6006110000	-2.2367270000	1.6856050000	C	2.1124870000	-2.0229640000	-1.8211390000
				C	-0.6005800000	-2.7786580000	0.3524800000	C	2.8068850000	-0.8174380000	-1.8203360000
				C	-1.8282530000	-2.3438330000	-0.2330330000	C	3.4030060000	-0.3564110000	-0.6077000000
								C	3.2545870000	1.0565660000	-0.6075220000
								C	2.5757090000	1.3837360000	-1.8203480000
								C	-2.7514070000	-0.9883870000	-1.8205640000
								C	-1.2704110000	-2.6330310000	-1.8207220000
								C	-2.9626650000	-1.7119740000	-0.6079760000
								C	-2.0119200000	-2.7677720000	-0.6081630000
								C	-3.4030060000	0.3564110000	0.6077000000
								C	-3.2545870000	-1.0565660000	0.6075220000
								C	-2.8068850000	0.8174380000	1.8203360000
								C	-2.5757090000	-1.3837360000	1.8203480000



**Table 3. Continued.**

7			8			9					
S	3.1786870000	0.0242150000	1.9349550000	S	3.1391950000	-0.3033060000	2.3547730000	S	3.1151960000	2.7266290000	-1.1475950000
S	3.1791900000	-1.6890840000	-0.9466200000	S	3.1391910000	-2.3547780000	-0.3033070000	S	3.1206350000	1.9494300000	2.2161720000
S	3.1791530000	1.6649030000	-0.9885380000	S	-3.1391500000	-1.8789230000	1.4505080000	S	-3.1551690000	2.8413770000	0.6607130000
S	-3.1791900000	1.6890850000	0.9466230000	S	-3.1391540000	-1.4505040000	-1.8789250000	S	-3.1363750000	0.2335740000	2.9245230000
S	-3.1786870000	-0.0242120000	-1.9349580000	S	3.1391910000	0.3033040000	-2.3547780000	S	3.1551760000	-2.8414510000	-0.6607400000
S	-3.1791530000	-1.6649070000	0.9885380000	S	3.1391940000	2.3547730000	0.3033030000	S	3.1363890000	-0.2335610000	-2.9246760000
C	-0.6024750000	2.0838590000	0.3417800000	S	-3.1391510000	1.8789240000	-1.4505020000	S	-3.1206330000	-1.9493710000	-2.2161250000
C	-1.8930480000	1.8775560000	-0.3143730000	S	-3.1391470000	1.4505050000	1.8789220000	S	-3.1451400000	1.4901930000	-2.5173470000
C	-0.6024880000	1.3780700000	1.5985080000	C	1.8610530000	0.9477430000	2.3700070000	S	-3.1151840000	-2.7265210000	1.1475280000
C	-1.8928220000	1.1734020000	-1.4977140000	C	0.6026800000	0.3729700000	2.7581090000	S	3.1452320000	-1.4903840000	2.5176550000
C	-0.6020720000	0.6959170000	-1.9922450000	C	0.6026220000	-1.0593470000	2.5737980000	C	1.8458680000	2.1999290000	-2.2962830000
C	-1.8931920000	0.7104610000	1.7632140000	C	1.8610130000	-1.5170520000	2.0529350000	C	0.5855240000	2.8134490000	-1.9690690000
C	-1.8931400000	-0.6660330000	1.7802070000	C	1.8610500000	-2.3700060000	0.9477430000	C	0.5814840000	3.3730500000	-0.6527490000
C	-0.6020690000	-0.7455340000	-1.9740250000	C	0.6026760000	-2.7581070000	0.3729690000	C	1.8388050000	3.1847940000	0.0223600000
C	-1.8927750000	-1.2105530000	-1.4677030000	C	0.6026180000	-2.5737980000	-1.0593470000	C	1.8409310000	2.8736250000	1.3695880000
C	-0.6024350000	-1.3374180000	1.6321720000	C	1.8610110000	-2.0529370000	-1.5170530000	C	1.8545350000	0.9718900000	3.0217860000
C	-1.8930450000	-1.8849460000	-0.2672900000	C	-0.6026830000	-2.5687750000	1.0706330000	C	0.5935140000	1.6659210000	3.0006300000
C	-0.6024000000	-2.0749830000	0.3938490000	C	-0.6026850000	-1.6862690000	2.2139350000	C	0.5858810000	2.7458040000	2.0627280000
C	0.6020700000	0.7455350000	1.9740250000	C	-1.8610530000	-1.0057440000	2.3461660000	C	-1.8839940000	3.1065300000	-0.5730100000
C	0.6020730000	-0.6959180000	1.9922470000	C	-1.8610520000	-2.5242660000	0.3786640000	C	-0.6303710000	3.4268440000	0.0577410000
C	0.6024020000	2.0749850000	-0.3938490000	C	-1.8610560000	-2.3461620000	-1.0057430000	C	-0.6280920000	3.1049800000	1.4515280000
C	1.8930430000	1.8849500000	0.2672900000	C	-0.6026890000	-2.2139330000	-1.6862700000	C	-1.8799320000	2.5394690000	1.8817690000
C	1.8927750000	1.2105520000	1.4677020000	C	-0.6026850000	-1.0706320000	-2.5687760000	C	-1.8725850000	1.4953870000	2.7886030000
C	0.6024750000	-2.0838590000	-0.3417800000	C	-1.8610530000	-0.3786630000	-2.5242670000	C	-0.6131310000	1.0006600000	3.2794440000
C	1.8930490000	-1.8775540000	0.3143720000	C	1.8610490000	-0.9477440000	-2.3700060000	C	-0.6029080000	-0.4242440000	3.4043850000
C	1.8928200000	-1.1734030000	1.4977170000	C	0.6026750000	-0.3729700000	-2.7581080000	C	-1.8544750000	-1.0145060000	3.0081060000
C	0.6024360000	1.3374180000	-1.6321720000	C	0.6026190000	1.0593460000	-2.5737960000	C	1.8840530000	-3.1063680000	0.5730220000
C	0.6024890000	-1.3780710000	-1.5985110000	C	1.8610120000	1.5170520000	-2.0529370000	C	0.6302990000	-3.4267290000	-0.0578030000
C	1.8931900000	-0.7104630000	-1.7632170000	C	1.8610520000	2.3700080000	-0.9477440000	C	0.6280380000	-3.1048200000	-1.4514710000
C	1.8931390000	0.6660330000	-1.7802070000	C	0.6026790000	2.7581100000	-0.3729710000	C	1.8799830000	-2.5393730000	-1.8817690000
				C	0.6026230000	2.5737960000	1.0593450000	C	1.8726220000	-1.4953720000	-2.7885600000
				C	1.8610140000	2.0529350000	1.5170520000	C	1.8544750000	1.0145210000	-3.0080580000
				C	-0.6026820000	2.5687760000	-1.0706320000	C	0.6028500000	0.4241800000	-3.4043410000
				C	-0.6026870000	1.6862700000	-2.2139320000	C	0.6130770000	-1.0006140000	-3.2794630000
				C	-1.8610560000	1.0057440000	-2.3461590000	C	-1.8408780000	-2.8736600000	-1.3696630000
				C	-1.8610490000	2.5242730000	-0.3786630000	C	-0.5859330000	-2.7458850000	-2.0627730000
				C	-1.8610530000	2.3461630000	1.0057450000	C	-0.5935840000	-1.6659160000	-3.0007370000
				C	-0.6026840000	2.2139330000	1.6862690000	C	-1.8544760000	-0.9719720000	-3.0219410000
				C	-0.6026810000	1.0706330000	2.5687750000	C	-1.8643620000	0.4055240000	-3.1427040000
				C	-1.8610480000	0.3786640000	2.5242720000	C	-0.6135970000	1.1106030000	-3.2440970000
								C	-0.6224870000	2.3367670000	-2.5075320000
								C	-1.8800610000	2.5655680000	-1.8457620000
								C	-1.8458680000	-2.1999810000	2.2962960000
								C	-1.8387660000	-3.1848340000	-0.0223460000
								C	-0.5855800000	-2.8134560000	1.9691500000
								C	-0.5815350000	-3.3730600000	0.6527050000
								C	0.6135230000	-1.1106500000	3.2440760000
								C	0.6224100000	-2.3367210000	2.5075650000
								C	1.8643500000	-0.4054770000	3.1426820000
								C	1.8800540000	-2.5655560000	1.8457090000

**Table 3. Continued.**

10			11			12					
Se	3.2967800000	0.5552470000	-1.9836720000	Se	-3.2986860000	-1.4140040000	-2.1418610000	Se	-3.2642010000	1.5747430000	-2.6424750000
Se	3.2966870000	1.4408680000	1.4727150000	Se	-3.2986850000	-2.1418620000	1.4140040000	Se	-3.2645900000	-2.0265940000	-2.3134900000
Se	3.2968200000	-1.9961880000	0.5110450000	Se	3.2986370000	-2.5150720000	-0.5150260000	Se	3.2640060000	-0.2799540000	-3.0626570000
Se	-3.2966870000	-1.4408680000	-1.4727140000	Se	3.2986370000	-0.5150250000	2.5150710000	Se	3.2638310000	-3.0002030000	-0.6811030000
Se	-3.2967800000	-0.5552470000	1.9836720000	Se	-3.2986860000	1.4140040000	2.1418640000	Se	-3.2640070000	0.2799540000	3.0626570000
Se	-3.2968200000	1.9961880000	-0.5110450000	Se	-3.2986870000	2.1418640000	-1.4140060000	Se	-3.2638310000	3.0002040000	0.6811030000
C	-0.6027480000	-1.9038310000	-0.9134380000	Se	3.2986360000	2.5150760000	0.5150260000	Se	3.2645900000	2.0265940000	2.3134900000
C	-1.8863830000	-1.9202660000	-0.2143420000	Se	3.2986370000	0.5150250000	-2.5150720000	Se	3.2644270000	2.8271120000	-1.2128240000
C	-0.6027070000	-0.8709410000	-1.9236870000	C	-1.8792810000	-0.1738490000	-2.5618090000	Se	3.2642010000	-1.5747430000	2.6424760000
C	-1.8864790000	-1.5810260000	1.1111960000	C	-0.6081000000	-0.8727350000	-2.6175680000	Se	-3.2644260000	-2.8271120000	1.2128240000
C	-0.6027470000	-1.2307920000	1.7164060000	C	-0.6081730000	-2.0640610000	-1.8310560000	C	-1.8553670000	2.6262900000	-1.8787980000
C	-1.8864150000	-0.1718150000	-1.9240440000	C	-1.8793270000	-2.2874750000	-1.1662010000	C	-0.6069490000	2.3376110000	-2.5204700000
C	-1.8862420000	1.1456230000	-1.5550230000	C	-1.8792800000	-2.5618130000	0.1738480000	C	-0.6071130000	1.1037610000	-3.2554580000
C	-0.6026820000	0.1606580000	2.1050940000	C	-1.8793270000	-1.1662010000	2.2874710000	C	-1.8556470000	0.4021950000	-3.2036120000
C	-1.8862470000	0.7742140000	1.7696600000	C	-0.6081720000	-1.8310570000	2.0640580000	C	-1.8557790000	-0.9752370000	-3.0776950000
C	-0.6026890000	1.7430290000	-1.1919480000	C	-0.6081000000	-2.6175720000	0.8727340000	C	-1.8559050000	-2.9228780000	-1.3722610000
C	-1.8862570000	1.7525300000	0.8131370000	C	1.8794150000	-1.9340020000	-1.6888290000	C	-0.6074670000	-2.7552790000	-2.0559900000
C	-0.6026170000	2.1015620000	0.2075180000	C	0.6081050000	-2.4673170000	-1.2334910000	C	-0.6074290000	-1.6749550000	-3.0018710000
C	0.6026820000	-0.1606580000	-2.1050940000	C	0.6081050000	-2.7539210000	0.1649620000	C	1.8553740000	1.0198600000	-3.0634180000
C	0.6027470000	1.2307920000	-1.7164060000	C	1.8795350000	-2.4431560000	0.7931590000	C	0.6069590000	0.4093220000	-3.4130830000
C	0.6026170000	-2.1015620000	-0.2075180000	C	1.8794150000	-1.6888300000	1.9340010000	C	0.6067880000	-1.0228900000	-3.2828420000
C	1.8862570000	-1.7525300000	-0.8131370000	C	0.6081050000	-1.2334910000	2.4673160000	C	1.8552120000	-1.5584700000	-2.8287010000
C	1.8862470000	-0.7742140000	-1.7696600000	C	0.6081050000	0.1649620000	2.7539190000	C	1.8550470000	-2.5988540000	-1.9171550000
C	0.6027480000	1.9038310000	0.9134380000	C	1.8795350000	0.7931590000	2.4431530000	C	0.6066930000	-3.1197870000	-1.4441430000
C	1.8863830000	1.9202660000	0.2143420000	C	-1.8792800000	0.1738470000	2.5618120000	C	0.6068000000	-3.4378300000	-0.0436540000
C	1.8864790000	1.5810260000	-1.1111960000	C	-0.6081000000	0.8727330000	2.6175710000	C	1.8552840000	-3.1715250000	0.6075800000
C	0.6026890000	-1.7430290000	1.1919480000	C	-0.6081720000	2.0640570000	1.8310550000	C	-1.8553740000	-1.0198600000	3.0634180000
C	0.6027070000	0.8709420000	1.9236870000	C	-1.8793280000	2.2874690000	1.1662000000	C	-0.6069590000	-0.4093220000	3.4130830000
C	1.8864150000	0.1718150000	1.9240440000	C	-1.8792810000	2.5618090000	-0.1738480000	C	-0.6067880000	1.0208900000	3.2828420000
C	1.8862420000	-1.1456230000	1.5550230000	C	-1.8793280000	1.1662010000	-2.2874730000	C	-1.8552120000	1.5584700000	2.8287000000
				C	-0.6081730000	1.8310560000	-2.0640590000	C	-1.8550470000	2.5988540000	1.9171550000
				C	-0.6081000000	2.6175700000	-0.8727340000	C	-1.8552840000	3.1715260000	-0.6075800000
				C	1.8794150000	1.9340010000	1.6888280000	C	-0.6068000000	3.4378300000	0.0436540000
				C	0.6081030000	2.4673150000	1.2334900000	C	-0.6066920000	3.1197870000	1.4441430000
				C	0.6081040000	2.7539200000	-0.1649630000	C	1.8557790000	0.9752360000	3.0776950000
				C	1.8795350000	2.4431550000	-0.7931600000	C	0.6074290000	1.6749550000	3.0018710000
				C	1.8794150000	1.6888280000	-1.9340000000	C	0.6074670000	2.7552790000	2.0559900000
				C	0.6081040000	1.2334900000	-2.4673150000	C	1.8559050000	2.9228780000	1.3722610000
				C	0.6081050000	-0.1649630000	-2.7539190000	C	1.8558550000	3.2292580000	0.0233960000
				C	1.8795350000	-0.7931600000	-2.4431550000	C	0.6073560000	3.3729400000	-0.6652620000
								C	0.6072940000	2.8067650000	-1.9851060000
								C	1.8555530000	2.2083370000	-2.3556310000
								C	1.8553670000	-2.6262900000	1.8787980000
								C	1.8556460000	-0.4021950000	3.2036120000
								C	0.6069490000	-2.3376110000	2.5204700000
								C	0.6071130000	-1.1037610000	3.2554580000
								C	-0.6073560000	-3.3729400000	0.6652620000
								C	-0.6072940000	-2.8067650000	1.9851060000
								C	-1.8558550000	-3.2292580000	-0.0233960000
								C	-1.8555530000	-2.2083370000	2.3556310000

#### 4. Optimised 1- Anion Geometries

1			2			3					
C	-0.9437720000	-1.9047720000	-0.6091730000	C	2.8105690000	-0.4559130000	1.8242710000	C	-3.4343200000	0.8054750000	-1.8244180000
C	-1.6169210000	-1.4514690000	-1.8219560000	C	2.7676290000	0.3379350000	0.6139210000	C	-3.1116570000	1.5222990000	-0.6150800000
C	0.4958680000	-2.0666980000	-0.6088790000	C	2.2313080000	1.6710140000	0.6139930000	C	-2.2275300000	2.6526570000	-0.6148930000
C	-2.1625890000	-0.2004180000	-1.8229870000	C	1.7128800000	2.2737470000	1.8243120000	C	-1.6098600000	3.1391240000	-1.8241900000
C	-2.0376090000	0.6031390000	-0.6114720000	C	0.4559130000	2.8105700000	1.8242710000	C	-0.2950240000	3.5140870000	-1.8242560000
C	1.2535160000	-1.7750660000	-1.8215300000	C	-0.3379350000	2.7676290000	0.6139210000	C	2.4882870000	2.5003850000	-1.8242780000
C	2.0644320000	-0.6771900000	-1.8224010000	C	-1.6710140000	2.2313080000	0.6139930000	C	1.8350200000	2.9376680000	-0.6149730000
C	-1.1774480000	1.7688530000	-0.6126340000	C	-2.2737470000	1.7128800000	1.8243120000	C	0.4864690000	3.4284370000	-0.6150020000
C	-0.4470810000	2.1229610000	-1.8252890000	C	0.3963440000	2.7596250000	-0.6139250000	C	-2.3049840000	2.6699950000	1.8240750000
C	2.1210850000	0.1342240000	-0.6109230000	C	1.7178220000	2.1952300000	-0.6139450000	C	-1.6223480000	3.0601220000	0.6148730000
C	0.9092750000	1.9703440000	-1.8249450000	C	2.3095570000	1.6643770000	-1.8243040000	C	-0.2425370000	3.4544500000	0.6147310000
C	1.5417560000	1.4619840000	-0.6121700000	C	-0.3963440000	2.8195270000	-1.8243310000	C	0.5430920000	3.4851270000	1.8239420000
C	1.1774480000	-1.7688530000	0.6126350000	C	-1.6643770000	2.3095570000	-1.8243040000	C	1.8277610000	3.0169930000	1.8240730000
C	2.0376100000	-0.6031390000	0.6114720000	C	-2.1952300000	1.7178220000	-0.6139450000	C	2.4098310000	2.4884410000	0.6148040000
C	-1.5417560000	-1.4619850000	0.6121700000	C	-2.7596250000	0.3963440000	-0.6139250000	C	3.2121490000	1.2986170000	-1.8248370000
C	-0.9092750000	-1.9703440000	1.8249450000	C	-2.8195270000	-0.3963440000	-1.8243300000	C	3.4835540000	0.5609010000	1.8242270000
C	0.4470810000	-2.1229610000	1.8252890000	C	-2.8105690000	0.4559130000	1.8242710000	C	3.2049840000	-2.6699950000	-1.8240750000
C	0.9437720000	1.9047720000	0.6091730000	C	-2.7676290000	-0.3379350000	0.6139210000	C	1.6223480000	-3.0601220000	-0.6148730000
C	1.6169210000	1.4514690000	1.8219560000	C	-2.2313080000	-1.6710140000	0.6139930000	C	0.2425370000	-3.4544500000	-0.6147310000
C	2.1625900000	0.2004180000	1.8229870000	C	-1.7128800000	-2.2737470000	1.8243120000	C	-0.5430920000	-3.4851270000	-1.8249420000
C	-2.1210850000	-0.1342240000	0.6109230000	C	-0.4559130000	-2.8105700000	1.8242710000	C	-1.8277610000	-3.0169930000	-1.8240730000
C	-0.4958680000	2.0666980000	0.6088790000	C	0.3379350000	-2.7676290000	0.6139210000	C	-3.4835540000	-0.5609010000	-1.8242270000
C	-1.2535160000	1.7750660000	1.8215300000	C	1.6710140000	-2.2313080000	0.6139930000	C	-3.2121490000	-1.2986170000	-0.6148370000
C	-2.0644320000	0.6771900000	1.8224000000	C	2.2737470000	-1.7128800000	1.8243120000	C	-2.4098310000	-2.4884410000	-0.6148040000
H	-1.5351110000	-2.0112790000	-2.7523470000	C	-0.3963440000	-2.7596250000	-0.6139250000	C	0.2950240000	-3.5140870000	1.8242560000
H	-2.5162120000	0.2394970000	-2.7542180000	C	-1.7178220000	-2.1952300000	-0.6139450000	C	-0.4864690000	-3.4284370000	0.6150020000
H	1.0485140000	-2.3020890000	-2.7520870000	C	-2.3095570000	-1.6643770000	-1.8243040000	C	-1.8350190000	-2.9376680000	0.6149730000
H	2.5075600000	-0.3275550000	-2.7536050000	C	0.3963440000	-2.8195270000	-1.8243310000	C	-2.4882870000	-2.5003850000	1.8242780000
H	-0.9719230000	2.3300330000	-2.7566240000	C	1.6643770000	-2.3095570000	-1.8243040000	C	-3.2523060000	-1.3665140000	1.8242080000
H	1.4677340000	2.0557590000	-2.7558380000	C	2.1952300000	-1.7178220000	-0.6139450000	C	-3.4129580000	-0.5971080000	0.6147910000
H	-1.4677340000	-2.0557590000	2.7558380000	C	2.7596250000	-0.3963440000	-0.6139250000	C	-3.3620820000	0.8371230000	0.6146100000
H	0.9719230000	-2.3300330000	2.7566240000	C	2.8195270000	0.3963440000	-1.8243300000	C	-3.1482810000	1.5937270000	1.8238180000
H	1.5351110000	2.0112790000	2.7523470000	H	3.1174880000	-0.0052970000	2.7656980000	C	3.4343200000	-0.8054750000	1.8244180000
H	2.5162120000	-0.2394970000	2.7542180000	H	2.2460890000	2.1605740000	2.7657560000	C	1.6098600000	-3.1391240000	1.8241900000
H	-1.0485140000	2.3020880000	2.7520870000	H	0.0052970000	3.1174880000	2.7656980000	C	3.1116570000	-1.5222990000	0.6150800000
H	-2.5075600000	0.3275540000	2.7536050000	H	-2.1605740000	2.2460890000	2.7657560000	C	2.2275300000	-2.6526570000	0.6148930000
				H	2.2075990000	2.1999650000	-2.7656900000	C	3.4129580000	0.5971080000	-0.6147910000
				H	0.0607630000	3.1167620000	-2.7657220000	C	3.3620820000	-0.8371230000	-0.6146100000
				H	-2.1999650000	2.2075990000	-2.7656900000	C	3.2523060000	1.3665140000	-1.8242080000
				H	-3.1167620000	0.0607630000	-2.7657220000	C	3.1482810000	-1.5937270000	-1.8238180000
				H	-3.1174880000	0.0052970000	2.7656980000	H	-3.5048390000	1.3375240000	-2.7697650000
				H	-2.2460890000	-2.1605740000	2.7657560000	H	-2.1435270000	3.0803900000	-2.7694180000
				H	-0.0052970000	-3.1174880000	2.7656980000	H	0.1892490000	3.7458230000	-2.7695110000
				H	2.1605740000	-2.2460890000	2.7657560000	H	2.2663470000	2.9887680000	-2.7697490000
				H	-2.2075990000	-2.1999650000	-2.7656900000	H	-2.0488110000	3.1411060000	2.7696570000
				H	-0.0607630000	-3.1167620000	-2.7657220000	H	0.0765160000	3.7508300000	2.7691720000
				H	2.1999650000	-2.2075990000	-2.7656900000	H	2.3554880000	2.9199640000	2.7694860000
				H	3.1167620000	-0.0607630000	-2.7657220000	H	3.5923350000	1.0867300000	2.7694170000
								H	2.0488110000	-3.1411060000	-2.7696570000
								H	-0.0765160000	-3.7508300000	-2.7691720000
								H	-2.3554880000	-2.9199640000	-2.7694860000
								H	-3.5923350000	-1.0867300000	-2.7694170000
								H	-0.1892490000	-3.7458230000	-2.7695110000
								H	-2.2663470000	-2.9887680000	2.7697490000
								H	-3.6221600000	-0.9774790000	2.7695160000
								H	-3.5451600000	1.2323220000	2.7691100000
								H	3.5048390000	-1.3375240000	2.7697650000
								H	2.1435270000	-3.0803900000	2.7694180000
								H	3.6221600000	0.9774790000	-2.7695160000
								H	3.5451600000	-1.2323220000	-2.7691100000

**Table 4. Continued.**

4			5			6					
O	-2.7533390000	-0.8320810000	-1.3254490000	O	-2.6976750000	-1.2786030000	1.5378180000	O	1.8657060000	1.6799990000	2.6514160000
O	-2.7532190000	-0.7320800000	1.3837880000	O	-2.6976690000	1.5379130000	1.2784620000	O	-1.0219860000	2.2946500000	2.6518950000
O	-2.7534880000	1.5634510000	-0.0579000000	O	2.6975270000	0.1836790000	1.9910560000	O	0.5218880000	2.4576460000	-2.6509430000
O	2.7532190000	0.7320800000	-1.3837880000	O	2.6976170000	1.9909660000	-0.1835490000	O	-2.1744870000	1.2561330000	-2.6510520000
O	2.7533390000	0.8320810000	1.3254490000	O	-2.6975330000	1.2785550000	-1.5380320000	O	-0.5218880000	-2.4576460000	2.6509430000
O	2.7534880000	-1.5634510000	0.0579000000	O	-2.6975380000	-1.5379380000	-1.2786910000	O	2.1744870000	-1.2561330000	2.6510520000
C	0.5882300000	1.6015520000	-1.4732620000	O	2.6977110000	-0.1836540000	-1.9908370000	O	1.0219860000	-2.2946500000	-2.6518950000
C	1.8496720000	1.6064290000	-0.7461740000	O	2.6976210000	-1.9909250000	0.1837820000	O	2.4970070000	0.2626710000	-2.6511520000
C	0.5882400000	0.3170750000	-2.1527170000	C	-1.8326360000	-2.1681040000	0.8883720000	O	-1.8657060000	-1.6799990000	-2.6514160000
C	1.8495630000	1.6565950000	0.6250290000	C	-0.5990440000	-2.2863970000	1.6340820000	O	-2.4970070000	-0.2626710000	2.6511520000
C	0.58851480000	1.7052910000	1.3501220000	C	-0.5989580000	-1.1888110000	2.5460940000	C	2.7474750000	0.9792810000	1.8228500000
C	1.8493750000	-0.2866190000	-1.7475570000	C	-1.8325820000	-0.4775890000	2.2936340000	C	2.9681950000	1.7227250000	0.6073210000
C	1.8497100000	-1.4488200000	-1.0177960000	C	-1.8327050000	0.8884350000	2.1680000000	C	2.0231990000	2.7721390000	0.6075060000
C	0.5884440000	0.4751880000	2.1240210000	C	-1.8325180000	2.2937180000	0.4774970000	C	1.2609130000	2.6300660000	1.8229670000
C	1.8494530000	-0.1565870000	1.7637300000	C	-0.5989220000	2.5461180000	1.1887800000	C	-0.0828520000	2.9161140000	1.8232150000
C	0.5885520000	-2.0766260000	-0.6503160000	C	-0.5990990000	1.6341020000	2.2863690000	C	-2.1126000000	2.0130890000	1.8234060000
C	1.8497140000	-1.3693370000	1.1220640000	C	1.8324780000	-0.9044510000	2.1611140000	C	-2.0118560000	2.7816560000	0.6074670000
C	0.5885630000	-2.0226150000	0.8021070000	C	0.5987400000	-0.4609100000	2.7709180000	C	-0.7216810000	3.3557990000	0.6076510000
C	-0.5884440000	-0.4751880000	-2.1240210000	C	0.5987540000	0.9600980000	2.6406510000	C	1.6467570000	2.4078350000	-1.8222090000
C	-0.5881480000	-1.7052910000	-1.3501220000	C	1.8324960000	1.2844330000	1.9593640000	C	1.3884550000	3.1386510000	-0.6064480000
C	-0.5885630000	2.0226150000	-0.8021070000	C	1.8325160000	2.1610500000	0.9045400000	C	0.0072530000	3.4330930000	-1.8224040000
C	-1.8497140000	1.3693370000	-1.1220640000	C	0.5988210000	2.7708990000	0.4609390000	C	-0.5259290000	2.8711000000	-1.8225530000
C	-1.8494530000	0.1565870000	-1.7637300000	C	0.5989030000	2.6406270000	-0.9600640000	C	-1.7807640000	2.3113080000	-1.8224450000
C	-0.5882300000	-1.6015520000	1.4732620000	C	1.8326390000	1.9593000000	-1.2843460000	C	-2.5558270000	2.2909720000	-0.6067620000
C	-1.8496720000	-1.6064290000	0.7461740000	C	-1.8325770000	2.1680810000	-0.8885280000	C	-3.2618090000	1.0679070000	-0.6070540000
C	-1.8495630000	-1.6565950000	-0.6250290000	C	-0.5989300000	2.2863930000	-1.6341280000	C	-2.8911140000	0.3870690000	-1.8227600000
C	-0.5885520000	2.0766260000	0.6503160000	C	-0.5987480000	1.1888040000	-2.5461460000	C	-1.6467570000	-2.4078350000	1.8222090000
C	-0.5882400000	-0.3170750000	2.1527170000	C	-1.8323750000	0.4775630000	-2.2937920000	C	-1.3884550000	-3.1386510000	0.6064480000
C	-1.8493750000	0.2866190000	1.7475570000	C	-1.8325060000	-0.8884640000	-2.1681760000	C	-0.0072530000	-3.4330930000	0.6064040000
C	-1.8497100000	1.4488200000	1.0177960000	C	-1.8324400000	-2.2937130000	-0.4776540000	C	0.5259290000	-2.8711000000	1.8225530000
				C	-0.5987840000	-2.5461230000	-1.1888350000	C	1.7807640000	-2.3113080000	1.8224450000
				C	-0.5988740000	-1.6341080000	-2.2864200000	C	2.8911140000	-0.3870690000	1.8227600000
				C	1.8326620000	0.9044700000	-2.1609550000	C	3.2618090000	-1.0679070000	0.6070540000
				C	0.5989810000	0.4609170000	-2.7708680000	C	2.5558270000	-2.2909720000	0.6067620000
				C	0.5990020000	-0.9600900000	-2.6405980000	C	0.0828520000	-2.9161140000	-1.8232150000
				C	1.8326960000	-1.2844280000	-1.9592230000	C	0.7216810000	-3.3557990000	-0.6076510000
				C	1.8326250000	-2.1610190000	-0.9043810000	C	2.0118560000	-2.7816560000	-0.6074670000
				C	0.5989010000	-2.7708870000	-0.4608870000	C	2.1126000000	-2.0130890000	-1.8234060000
				C	0.5988530000	-2.6406220000	0.9601240000	C	2.7983820000	-0.8225180000	-1.8226440000
				C	1.8325510000	-1.9592840000	1.2845120000	C	3.4138000000	-0.3509540000	-0.6070470000
								C	3.2662910000	1.0534750000	-0.6068810000
								C	2.5662820000	1.3869010000	-1.8226760000
								C	-2.7474750000	-0.9792810000	-1.8228500000
								C	-1.2609130000	-2.6300660000	-1.8229670000
								C	-2.9681950000	-1.7227250000	-0.6073210000
								C	-2.0231990000	-2.7721390000	-0.6075060000
								C	-3.4138000000	0.3509540000	0.6070470000
								C	-3.2662910000	-1.0534750000	0.6068810000
								C	-2.7983820000	0.8225180000	-1.8226440000
								C	-2.5662820000	-1.3869010000	1.8226760000

**Table 4. Continued.**

7			8			9					
S	3.1613130000	0.0185900000	-1.9283900000	S	3.1544870000	-2.3591090000	-0.4761800000	S	3.1448680000	1.3789460000	2.5901320000
S	3.1615760000	1.6617290000	0.9803720000	S	3.1544860000	0.4761800000	-2.3591100000	S	-3.1300320000	-0.4063230000	2.9212030000
S	3.1615200000	-1.6804070000	0.9483040000	S	-3.1544070000	-1.3312520000	-2.0042700000	S	-3.1448650000	-1.3789380000	-2.5901170000
S	-3.1615760000	-1.6617290000	-0.9803730000	S	-3.1544060000	2.0042710000	-1.3312510000	S	-3.1384600000	-2.8975510000	0.5192380000
S	-3.1613130000	-0.0185910000	1.9283910000	S	3.1544860000	2.3591090000	0.4761810000	S	3.1313110000	-2.6491390000	-1.2982260000
S	-3.1615200000	1.6804080000	-0.9483040000	S	3.1544860000	-0.4761810000	2.3591080000	S	3.1405190000	-2.0480260000	2.1094970000
C	-0.5939280000	-2.1083370000	-0.4029020000	S	-3.1544070000	1.3312490000	2.0042690000	S	-3.1313100000	2.6491290000	1.2982210000
C	-1.8736600000	-1.8925000000	0.2783680000	S	-3.1544080000	-2.0042680000	1.3312500000	S	-3.1405180000	2.0480190000	-2.1094890000
C	-0.5939050000	-1.3718530000	-1.6512540000	C	1.8657490000	-2.4185470000	0.7806240000	S	3.1384610000	2.8975610000	-0.5192400000
C	-1.8734590000	-1.2153850000	1.4761280000	C	0.6013510000	-2.7881370000	0.1663470000	S	3.1300340000	0.4063240000	-2.9212140000
C	-0.5937900000	-0.7443480000	2.0135130000	C	0.6013740000	-2.5056310000	-1.2345170000	C	1.8700240000	0.2493560000	3.1560820000
C	-1.8738260000	-0.6706400000	-1.7894190000	C	1.8657670000	-1.9267600000	-1.6578570000	C	1.8691970000	2.4794640000	1.9712260000
C	-1.8737380000	0.7047300000	-1.7758100000	C	1.8657490000	-0.7806240000	-2.4185470000	C	0.6155420000	0.9539950000	3.3043860000
C	-0.5938330000	0.7053870000	2.0271120000	C	0.6013510000	-0.1663470000	-2.7881390000	C	0.6150620000	2.2075120000	2.6387280000
C	-1.8733860000	1.1866370000	1.4986760000	C	0.6013730000	1.2345170000	-2.5056310000	C	-0.5992690000	-1.1706760000	3.2371020000
C	-0.5938230000	1.4029350000	-1.6239230000	C	1.8657660000	1.6578570000	-1.9267600000	C	-0.5973880000	0.2348120000	3.4347050000
C	-1.8737210000	1.8870060000	0.3146240000	C	-0.6013660000	-0.8985640000	-2.6444360000	C	-1.8565400000	-1.6532900000	2.7092830000
C	-0.5938360000	2.1163450000	-0.3622680000	C	-0.6014370000	-2.0890660000	-1.8536260000	C	-1.8533510000	0.8474150000	3.0611590000
C	0.5938340000	-0.7053870000	-2.0271120000	C	-1.8657540000	-2.2622800000	-1.1577970000	C	-1.8700240000	-3.2493570000	-3.1560870000
C	0.5937910000	0.7443490000	-2.0135160000	C	-1.8658960000	-0.1901920000	-2.5347900000	C	-0.6155450000	-0.9539930000	-3.3043890000
C	0.5938370000	-2.1163480000	0.3622680000	C	-1.8657520000	1.1577980000	-2.2622780000	C	-0.6150670000	-2.2075160000	-2.6387290000
C	1.8737200000	-1.8870080000	-0.3146240000	C	-0.6014370000	1.8536270000	-2.0890660000	C	-1.8691960000	-2.4794640000	-1.9712290000
C	1.8733860000	-1.1866370000	-1.4986760000	C	-0.6013660000	2.6444360000	-0.8985640000	C	-1.8666250000	-3.0839560000	-0.7334970000
C	0.5939280000	2.1083370000	0.4029020000	C	-1.8658940000	2.5347890000	-0.1901920000	C	-0.6097080000	-3.4398580000	-0.1123850000
C	1.8736600000	1.8924990000	-0.2783680000	C	1.8657480000	2.4185460000	-0.7806230000	C	-0.6059210000	-3.1935280000	1.2854070000
C	1.8734580000	1.2153860000	-1.4761290000	C	0.6013510000	2.7881380000	-0.1663460000	C	-1.8599000000	-2.6449150000	1.7533060000
C	0.5938240000	-1.4029340000	1.6239230000	C	0.6013730000	2.5056320000	1.2345190000	C	0.6010180000	-3.3390690000	-0.8400110000
C	0.5939050000	1.3718540000	1.6512570000	C	1.8657670000	1.9267620000	1.6578590000	C	0.5983620000	-2.7169990000	-2.1156760000
C	1.8738250000	0.6706410000	1.7894210000	C	1.8657490000	0.7806230000	2.4185450000	C	1.8538350000	-2.0638790000	-2.4149720000
C	1.8737380000	-0.7047300000	1.7758100000	C	0.6013510000	0.1663460000	2.7881360000	C	1.8585320000	-3.1706660000	-0.1452790000
				C	0.6013740000	-1.2345180000	2.5056320000	C	1.8622160000	-2.9314910000	1.2111880000
				C	1.8657670000	-1.6578600000	1.9267620000	C	0.6085380000	-2.8508230000	1.9282890000
				C	-0.6013660000	0.8985630000	2.6444350000	C	0.6118930000	-1.8297700000	2.9140710000
				C	-0.6014370000	2.0890670000	1.8536280000	C	1.8683710000	-1.1148180000	2.9651330000
				C	-1.8657530000	2.2622800000	1.1577990000	C	-1.8538350000	2.0638830000	2.4149750000
				C	-1.8658950000	0.1901910000	2.5347890000	C	-0.5983650000	2.7170010000	2.1156810000
				C	-1.8657540000	-1.1577980000	2.2622830000	C	-0.6010210000	3.3390730000	0.8400100000
				C	-0.6014370000	-1.8536260000	2.0890670000	C	-1.8585290000	3.1706690000	0.1452800000
				C	-0.6013660000	-2.6444350000	0.8985630000	C	-1.8622150000	2.9314960000	-1.2111930000
				C	-1.8658970000	-2.5347910000	0.1901910000	C	-0.6085420000	2.8508280000	-1.9282900000
								C	-0.6118970000	1.8297710000	-2.9140770000
								C	-1.8683680000	1.1148220000	-2.9651370000
								C	0.6059180000	3.1935230000	-1.2854040000
								C	0.6097050000	3.4398530000	0.1123820000
								C	1.8666260000	3.0839480000	0.7334970000
								C	1.8599020000	2.6449110000	-1.7533070000
								C	1.8565410000	1.6532870000	-2.7092780000
								C	0.5992660000	1.1706730000	-3.2371000000
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								C	1.8533520000	-0.8474170000	-3.0611560000

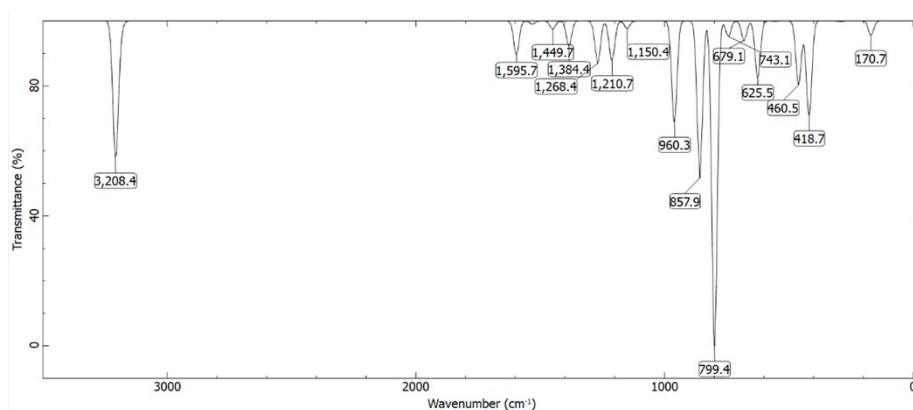
**Table 4. Continued.**

10				11				12			
Se	3.2798500000	-1.8607400000	0.8478290000	Se	-3.2825950000	-1.4526680000	-2.1044570000	Se	-3.2746080000	1.3855430000	-2.7664670000
Se	3.2790980000	0.1959820000	-2.0358680000	Se	-3.2825940000	-2.1044580000	1.4526670000	Se	-3.2740520000	-2.2028280000	-2.1734950000
Se	3.2793550000	1.6653160000	1.1876970000	Se	3.2825530000	-2.5157460000	-0.4601130000	Se	3.2753770000	-0.5041550000	-3.0517110000
Se	-3.2790980000	-0.1959820000	2.0358680000	Se	3.2825530000	-0.4601130000	2.5157460000	Se	3.2753810000	-3.0601860000	-0.4632930000
Se	-3.2798500000	1.8607400000	-0.8478290000	Se	-3.2825950000	1.4526680000	2.1044600000	Se	-3.2753770000	0.5041550000	3.0517110000
Se	-3.2793550000	-1.6653160000	-1.1876980000	Se	-3.2825950000	2.1044590000	-1.4526690000	Se	-3.2753810000	3.0601860000	0.4632930000
C	-0.5935100000	0.5284000000	2.0795610000	Se	3.2825520000	2.5157490000	0.4601130000	Se	3.2740520000	2.2028280000	2.1734950000
C	-1.8665630000	1.0839830000	1.6123220000	Se	3.2825520000	0.4601130000	-2.5157460000	Se	3.2745780000	2.7489230000	-1.4232140000
C	-0.5936420000	-0.9166880000	1.9429570000	C	-1.8615030000	-0.2236470000	-2.5694970000	Se	3.2746080000	-1.3855430000	2.7664670000
C	-1.8659780000	1.8768040000	0.4987160000	C	-0.6013170000	-0.9456420000	-2.6302630000	Se	-3.2745780000	-2.7489230000	1.4232140000
C	-0.5942880000	2.1410660000	-0.1779520000	C	-0.6012820000	-2.1248650000	-1.8164290000	C	-1.8578350000	2.4812680000	-2.0556750000
C	-1.8665020000	-1.3701810000	1.3753720000	C	-1.8616550000	-2.3240400000	-1.1203160000	C	-0.6060910000	2.1482790000	-2.6982930000
C	-1.8667030000	-1.9373770000	0.1320620000	C	-1.8615020000	-2.5695010000	0.2236460000	C	-0.6057430000	0.8754700000	-3.3363160000
C	-0.5943540000	1.5390500000	-1.4991760000	C	-1.8616550000	-1.1203160000	2.3240370000	C	-1.8571570000	0.1607170000	-3.2191160000
C	-1.8659970000	0.8547360000	-1.7428660000	C	-0.6012820000	-1.8164290000	2.1248620000	C	-1.8569850000	-1.1886300000	-2.9960360000
C	-0.5937570000	-2.0681200000	-0.5827360000	C	-0.6013170000	-2.6302660000	0.9456420000	C	-1.8570270000	-3.0113940000	-1.1479030000
C	-1.8668040000	-0.5056540000	-1.8752280000	C	1.8616630000	-1.9756870000	-1.6584910000	C	-0.6054670000	-2.9025890000	-1.8636950000
C	-0.5937490000	-1.2230130000	-1.7629390000	C	0.6012300000	-2.5283800000	-1.1909640000	C	-0.6053830000	-1.9026920000	-2.8773900000
C	0.5943540000	-1.5390500000	1.4991770000	C	0.6013220000	-2.7863430000	0.2183880000	C	1.8581200000	-3.7997770000	-3.1212910000
C	0.5942880000	-2.1410650000	0.1779520000	C	1.8617830000	-2.4349140000	0.8519170000	C	0.6066980000	0.1521210000	-3.4457740000
C	0.5937490000	1.2230130000	1.7629390000	C	1.8616640000	-1.6584920000	1.9756860000	C	0.6068430000	-1.2525580000	-3.2132150000
C	1.8668050000	0.5056540000	1.8752290000	C	0.6012300000	-1.1909650000	2.5283800000	C	1.8583440000	-1.7613470000	-2.6979290000
C	1.8659970000	-0.8547360000	1.7428670000	C	0.6013210000	0.2183870000	2.7863410000	C	1.8583900000	-2.7225000000	-1.7250170000
C	0.5935100000	-0.5284000000	-2.0795610000	C	1.8617830000	0.8519170000	2.4349120000	C	0.6067220000	-3.2308160000	-1.2095750000
C	1.8665630000	-1.0839830000	-1.6123220000	C	-1.8615020000	0.2236460000	2.5695020000	C	0.6066280000	-3.4436970000	0.1982330000
C	1.8659780000	-1.8768040000	-0.4987160000	C	-0.6013170000	0.9456410000	2.6302670000	C	1.8580370000	-3.1105220000	0.8414640000
C	0.5937570000	2.0681200000	0.5827360000	C	-0.6012820000	2.1248610000	1.8164270000	C	-1.8581200000	-0.7997770000	3.1212920000
C	0.5936420000	0.9166880000	-1.9429570000	C	-1.8616560000	2.3240340000	1.1203150000	C	-0.6066980000	-0.1521210000	3.4457740000
C	1.8665020000	1.3701810000	-1.3753720000	C	-1.8615040000	2.5694970000	-0.2236470000	C	-0.6068430000	1.2525580000	3.2132150000
C	1.8667030000	1.9373770000	-0.1320620000	C	-1.8616560000	1.1203150000	-2.3240380000	C	-1.8583440000	1.7613470000	2.6979290000
				C	-0.6012830000	1.8164290000	-2.1248640000	C	-1.8583900000	2.7225000000	1.7250170000
				C	-0.6013170000	2.6302640000	-0.9456420000	C	-1.8580370000	3.1105220000	-0.8414640000
				C	1.8616620000	1.9756860000	1.6584900000	C	-0.6066280000	3.4436970000	-0.1982330000
				C	0.6012290000	2.5283790000	1.1909640000	C	-0.6067220000	3.2308160000	1.2095750000
				C	0.6013200000	2.7863430000	-0.2183890000	C	1.8569850000	1.1886300000	2.9960360000
				C	1.8617820000	2.4349150000	-0.8519180000	C	0.6053830000	1.9026920000	2.8773900000
				C	1.8616620000	1.6584900000	-1.9756850000	C	0.6054670000	2.9025890000	1.8636950000
				C	0.6012290000	1.1909640000	-2.5283790000	C	1.8570270000	3.0113940000	1.1479030000
				C	0.6013210000	-0.2183890000	-2.7863420000	C	1.8572940000	3.2170250000	-0.2041680000
				C	1.8617830000	-0.8519180000	-2.4349140000	C	0.6056980000	3.3249230000	-0.9201640000
								C	0.6059220000	2.6693270000	-2.1841010000
								C	1.8576360000	2.0224970000	-2.5086820000
								C	1.8578350000	-2.4812680000	2.0556750000
								C	1.8571570000	-0.1607170000	3.2191160000
								C	0.6060910000	-2.1482790000	2.6982930000
								C	0.6057430000	-0.8754700000	3.3363160000
								C	-0.6056980000	-3.3249230000	0.9201640000
								C	-0.6059220000	-2.6693270000	2.1841010000
								C	-1.8572940000	-3.2170250000	0.2041680000
								C	-1.8576360000	-2.0224970000	2.5086820000

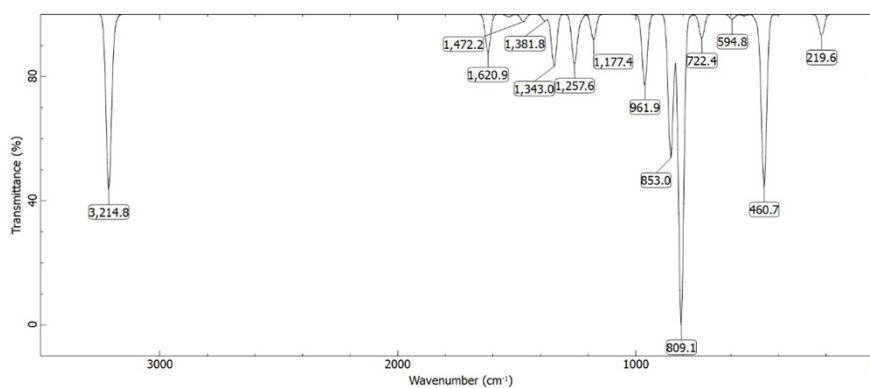
## 5. Frontier Molecular Orbitals

Entry	$\psi_{H-1}$	$\psi_H$	$\psi_L$	$\psi_{L+1}$
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				

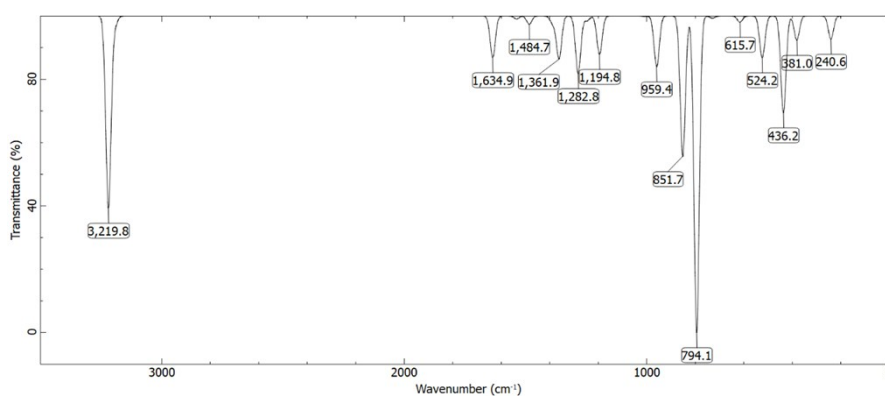
## 6. Vibrational Spectra



**Figure S2.** Infrared Spectrum of Optimized Compound 1 at the B3LYP/6-31+G(d) Level.

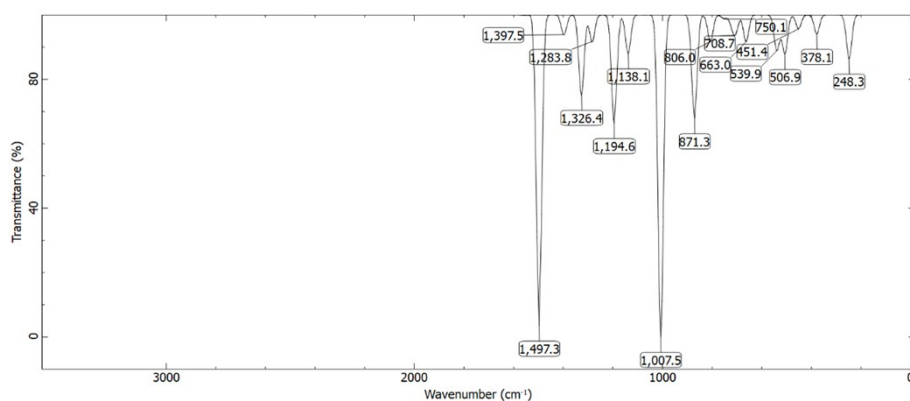


**Figure S3.** Infrared Spectrum of Optimized Compound 2 at the B3LYP/6-31+G(d) Level.

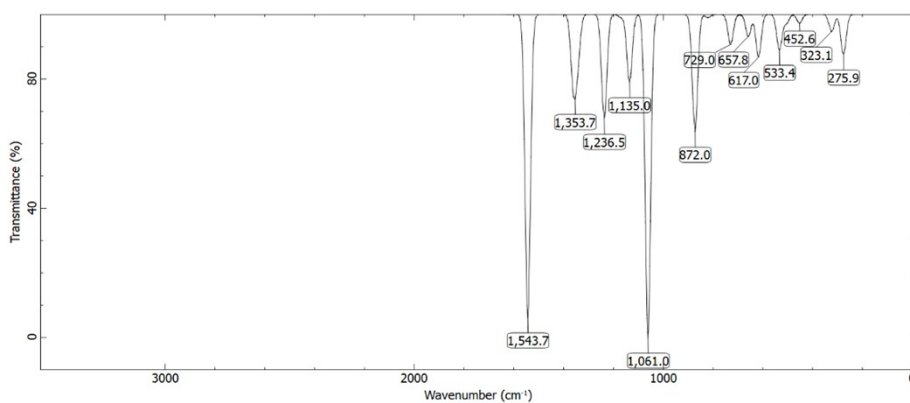


**Figure S4.** Infrared Spectrum of Optimized Compound 3 at the B3LYP/6-31+G(d) Level.

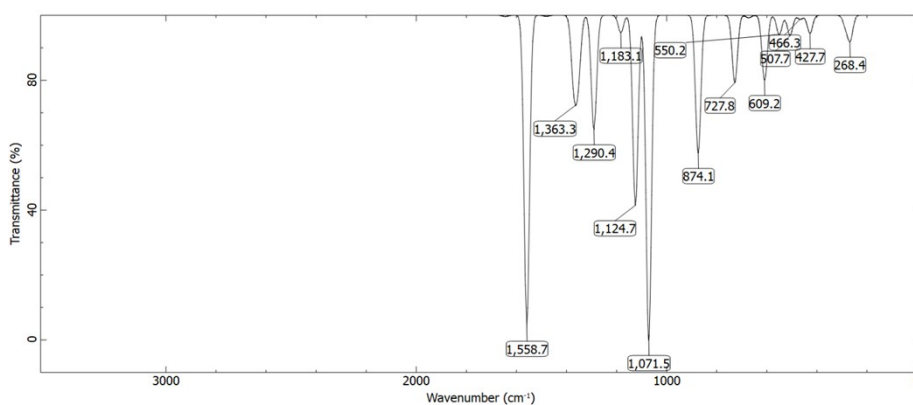




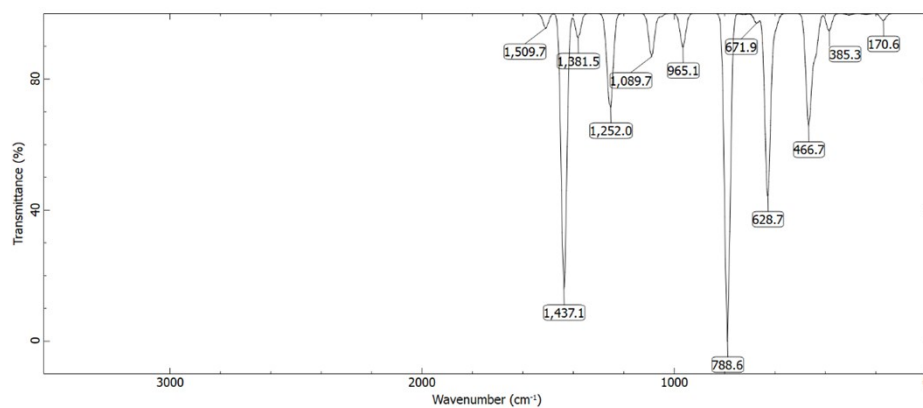
**Figure S5.** Infrared Spectrum of Optimized Compound 4 at the B3LYP/6-31+G(d) Level.



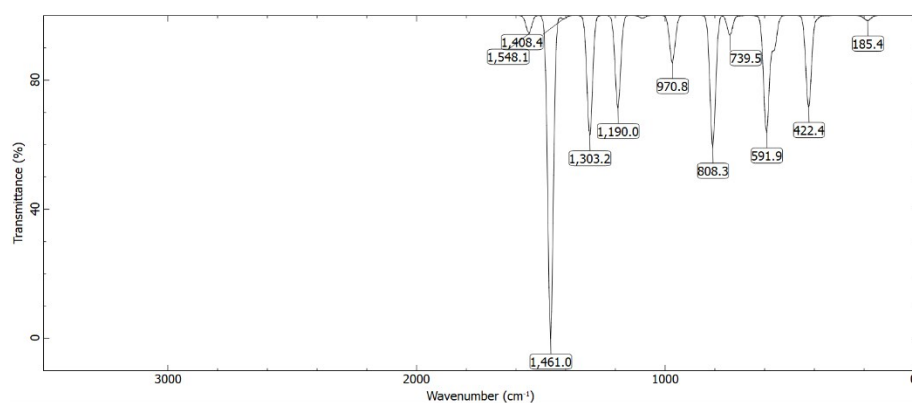
**Figure S6.** Infrared Spectrum of Optimized Compound 5 at the B3LYP/6-31+G(d) Level.



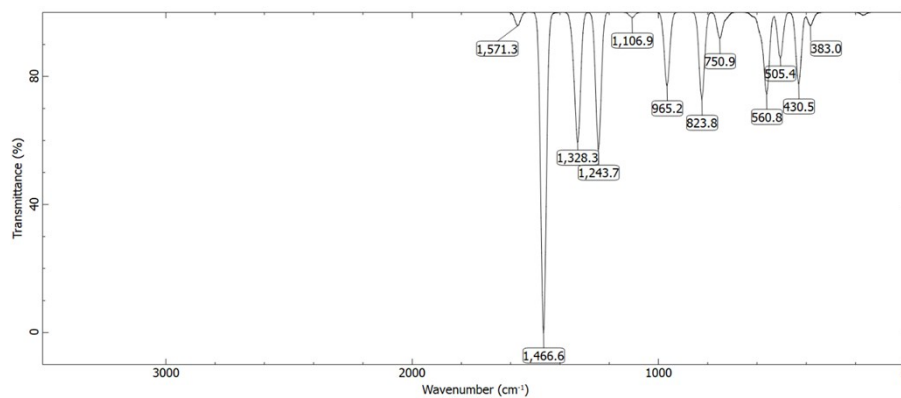
**Figure S7.** Infrared Spectrum of Optimized Compound 6 at the B3LYP/6-31+G(d) Level.



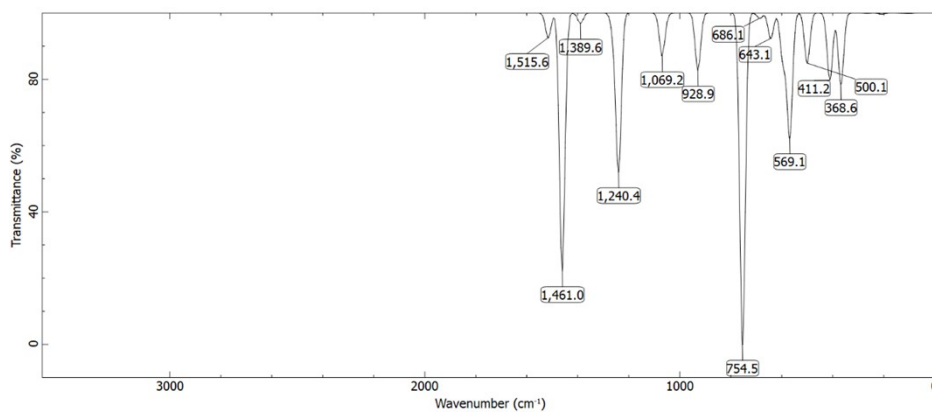
**Figure S8.** Infrared Spectrum of Optimized Compound 7 at the B3LYP/6-31+G(d) Level.



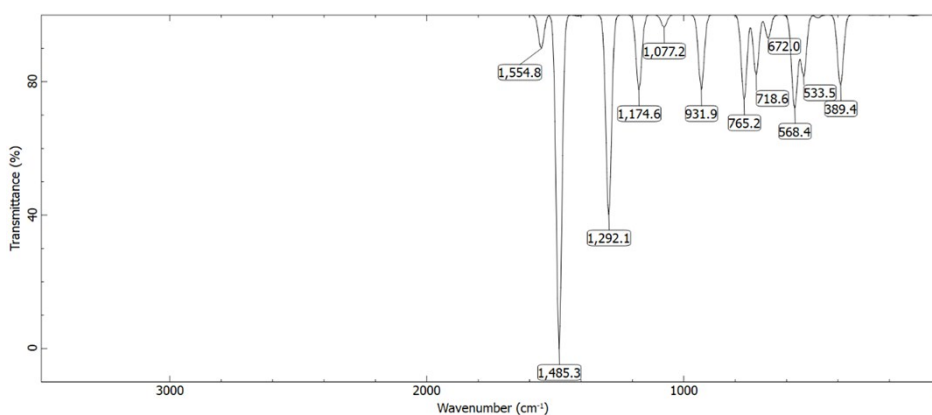
**Figure S9.** Infrared Spectrum of Optimized Compound 8 at the B3LYP/6-31+G(d) Level.



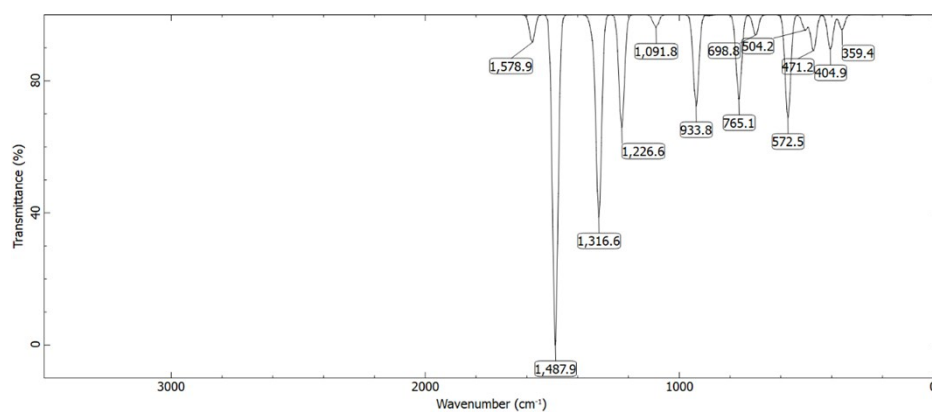
**Figure S10.** Infrared Spectrum of Optimized Compound 9 at the B3LYP/6-31+G(d) Level.



**Figure S11.** Infrared Spectrum of Optimized Compound 10 at the B3LYP/6-31+G(d) Level.



**Figure S12.** Infrared Spectrum of Optimized Compound 11 at the B3LYP/6-31+G(d) Level.



**Figure S13.** Infrared Spectrum of Optimized Compound 12 at the B3LYP/6-31+G(d) Level.

## 7. Hole and Electron Reorganisation Energies, Transfer Integrals and Rates

### 7.1 Integrals and rates

**Table 6.** The hole reorganisation energy ( $\lambda_h$ ), the hole transfer integrals ( $t_h$ ) and the rate of hole charge transfer ( $K_{CT_h} \times 10^{13} / s^{-1}$ ) with increasing intermolecular separation ( $d$ ) between 3.0 and 5.0 Å.

Entry	$\lambda_h$	$d=3.0 \text{ \AA}$		$d=3.5 \text{ \AA}$		$d=4.0 \text{ \AA}$		$d=4.5 \text{ \AA}$		$d=5.0 \text{ \AA}$	
		$t_h$	$K_{CT_h}$	$t_h$	$K_{CT_h}$	$t_h$	$K_{CT_h}$	$t_h$	$K_{CT_h}$	$t_h$	$K_{CT_h}$
1	401	29.4	0.007	18.9	0.003	12.0	0.001	7.48	0.000	4.49	0.000
2	295	70.5	0.139	36.9	0.038	19.0	0.010	9.80	0.003	5.03	0.001
3	230	60.3	0.216	30.5	0.055	15.8	0.015	8.16	0.004	4.22	0.001
4	447	13.9	0.001	6.94	0.000	3.54	0.000	1.77	0.000	0.95	0.000
5	303	40.8	0.042	21.0	0.012	10.9	0.003	5.58	0.001	2.72	0.000
6	211	35.2	0.093	18.5	0.026	9.66	0.007	4.90	0.002	2.45	0.000
7	195	188	3.215	102	0.894	55.8	0.283	30.2	0.083	16.2	0.024
8	138	37.8	0.269	18.4	0.063	9.12	0.016	4.49	0.004	2.18	0.001
9	112	3.67	0.004	2.59	0.002	-	-	-	-	-	-
10	395	167	0.256	92.1	0.073	50.3	0.023	27.3	0.007	14.7	0.002
11	280	54.8	0.100	26.8	0.024	13.6	0.006	7.21	0.002	3.67	0.000
12	86	17.0	0.114	-	-	-	-	-	-	-	-

**Table 7.** The electron reorganisation energy ( $\lambda_e$ ), the electron transfer integrals ( $t_e$ ) and the rate of electron charge transfer ( $K_{CT_e} \times 10^{13} / s^{-1}$ ) with increasing intermolecular separation ( $d$ ) between 3.0 and 5.0 Å.

Entry	$\lambda_e$	$d=3.0 \text{ \AA}$		$d=3.5 \text{ \AA}$		$d=4.0 \text{ \AA}$		$d=4.5 \text{ \AA}$		$d=5.0 \text{ \AA}$	
		$t_e$	$K_{CT_e}$	$t_e$	$K_{CT_e}$	$t_e$	$K_{CT_e}$	$t_e$	$K_{CT_e}$	$t_e$	$K_{CT_e}$
1	327	41.1	0.033	21.8	0.009	11.0	0.002	5.31	0.001	2.59	0.000
2	235	83.1	0.387	47.1	0.059	27.3	0.042	16.2	0.015	9.52	0.005
3	193	71.8	0.480	40.4	0.072	23.0	0.049	13.1	0.016	7.35	0.005
4	263	75.0	0.227	53.1	0.114	35.9	0.052	23.5	0.022	15.0	0.009
5	200	99.7	0.849	55.6	0.264	31.2	0.083	17.4	0.026	9.66	0.008
6	169	66.7	0.558	34.3	0.148	17.6	0.039	8.98	0.010	4.63	0.003
7	266	83.9	0.275	63.9	0.159	54.0	0.114	30.3	0.036	17.0	0.011
8	198	63.3	0.350	34.3	0.103	18.9	0.031	10.6	0.010	5.99	0.003
9	167	47.6	0.292	38.5	0.191	-	-	-	-	-	-
10	255	80.1	0.284	63.5	0.179	50.3	0.112	28.4	0.036	16.1	0.011
11	200	62.7	0.336	33.9	0.098	18.8	0.030	10.6	0.010	5.99	0.003
12	279	1.22	0.000	-	-	-	-	-	-	-	-

## 8. Hole and Electron Mobility Data

**Table 8.** Hole ( $\mu_h$ ) and electron ( $\mu_e$ ) mobilities ( $\mu / \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ ) between  $d = 3.0\text{-}4.0 \text{ \AA}$ .

Entry	$d=3.0 \text{ \AA}$		$d=3.5 \text{ \AA}$		$d=4.0 \text{ \AA}$	
	$\mu_h$	$\mu_e$	$\mu_h$	$\mu_e$	$\mu_h$	$\mu_e$
1	0.003	0.011	0.001	0.004	0.001	0.000
2	0.049	0.136	0.018	0.059	0.010	0.000
3	0.076	0.168	0.026	0.072	0.000	0.000
4	0.000	0.079	0.000	0.054	0.000	0.000
5	0.015	0.298	0.005	0.126	0.003	0.000
6	0.032	0.196	0.012	0.070	0.007	0.000
7	1.126	0.096	0.453	0.076	0.000	0.000
8	0.094	0.123	0.030	0.049	0.000	0.000
9	0.001	0.102	0.001	0.091	-	-
10	0.090	0.100	0.037	0.085	0.000	0.000
11	0.035	0.118	0.011	0.047	0.000	0.000
12	0.040	0.000	-	-	-	-