Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The role of electric field, peripheral chains, and magnetic effects on significant ^{1}H upfield shifts of the encapsulated molecules in chalcogen-bonded capsules.

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Theoretical Section

A. Analysis of the many-body interaction energy terms

The BSSE-corrected interaction energies (ΔE), deformation terms (D), the BSSE-corrected two- (Δ^2E) and three-body (Δ^3E) terms are:

$$\Delta E = E^{x_i x_j \cdots}_{X_i X_j \cdots}(X_i X_j \ldots.) - \sum_i E^{x_i x_j \cdots}_{X_i X_j \cdots}(X_i) + \sum_i D_{X_i}$$

$$D_{X_i} = E^{x_i}_{X_i X_j \cdots}(X_i) - E^{x_i}_{X_i}(X_i)$$

$$\Delta^2 E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i X_j, BSSE) = E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i X_j) - \left\{E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i) + E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_j)\right\}$$

$$\Delta^3 E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i X_j X_k, BSSE) = E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i X_j X_k) - \left\{E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i) + E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_j) + E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_k)\right\} - \left\{\Delta^2 E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i X_j) + \Delta^2 E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_i X_k) + \Delta^2 E^{x_1 x_2 \cdots}_{X_1 X_2 \cdots}(X_j X_k)\right\}$$

where, $E^s_G(M)$ refers to the total energy of the molecule *M* computed at the geometry *G* with basis set *s*.

B. Dipole moment (*μ*), linear polarizability (*α*) and first-order hyperpolarizability (*β*)

- The total dipole moment is calculated using the following equation:

$$\mu_{tot} = \left(\mu_x^2 + \mu_y^2 + \mu_z^2\right)^{\frac{1}{2}}$$

- Linear polarizability (*α*) is calculated using the following equation:

$$\alpha_{tot} = \frac{1}{3}\left(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}\right)$$

$$\Delta\alpha = \frac{1}{\sqrt{2}}\left[\left(\alpha_{xx} - \alpha_{yy}\right)^2 + \left(\alpha_{yy} - \alpha_{zz}\right)^2 + \left(\alpha_{zz} - \alpha_{xx}\right)^2 + 6\alpha_{xz}^2 + 6\alpha_{xy}^2 + 6\alpha_{yz}^2\right]^{\frac{1}{2}}$$

where: α_{xx}, α_{xy}, α_{yy}, α_{xz}, α_{yz}, α_{zz}, polarizability tensors

- First-order hyperpolarizability (*β*) is calculated using the following equation:

$$\langle\beta\rangle = \left[\left(\beta_{xxx} + \beta_{xyy} + \beta_{xzz}\right)^2 + \left(\beta_{yyy} + \beta_{yzz} + \beta_{yxx}\right)^2 + \left(\beta_{zzz} + \beta_{zxx} + \beta_{zyy}\right)^2\right]^{\frac{1}{2}}$$

where: β_{xxx}, β_{xxy}, β_{xyy}, β_{yyy}, β_{xxz}, β_{xyz}, β_{yyz}, β_{xzz}, β_{yzz}, β_{zzz} hyperpolarizability tensors

Table 1S Charges via the Mulliken, CM5 and NBO analyses q_x on the halogen (Br or I), q_Y on the chalcogen (Se and Te) of $\mathbf{A_x+A_x}$, and $\mathbf{RX+RX'@A_x+A_x}$, at M06-2X/6-31G(d,p) level of theory.

	Mulliken		CM5		NBO		Mulliken		CM5		NBO	
	X	X'	X	X'	X	X'	Y	Y'	Y	Y'	Y	Y'
$\mathbf{A_{Se}+A_{Se}}$							0.57	0.57	0.43	0.43	0.97	0.97
RBr+RBr@A_{Se}+A_{Se}	-0.16	-0.16	-0.07	-0.07	-0.08	-0.08	0.58	0.58	0.44	0.44	0.99	0.99
RBr+RI@A_{Se}+A_{Se}	-0.16	-0.19	-0.08	-0.01	-0.07	0.06	0.55	0.55	0.44	0.44	0.99	0.99
RI+RI@A_{Se}+A_{Se}	-0.18	-0.18	-0.01	-0.01	0.07	0.07	0.55	0.55	0.44	0.44	0.99	0.99
C_9H_{20}@A_{Se}+A_{Se}							0.58	0.58	0.44	0.44	0.98	0.98
$\mathbf{A_{Se}+A_{Te}}$							0.62	0.80	0.47	0.48	1.04	1.24
RBr+RBr@A_{Se}+A_{Te}	-0.16	-0.18	-0.07	-0.08	-0.06	-0.08	0.62	0.80	0.48	0.50	1.05	1.26
RI+RBr@A_{Se}+A_{Te}	-0.16	-0.15	0.00	-0.09	0.08	-0.08	0.62	0.80	0.47	0.49	1.05	1.26
RBr+RI@A_{Se}+A_{Te}	-0.14	-0.19	-0.06	-0.02	-0.06	0.05	0.62	0.80	0.47	0.50	1.05	1.26
RI+RI@A_{Se}+A_{Te}	-0.17	-0.19	-0.02	-0.01	0.06	0.05	0.62	0.81	0.47	0.50	1.04	1.26
C_9H_{20}@A_{Se}+A_{Te}							0.62	0.80	0.47	0.50	1.04	1.25
$\mathbf{A_{Te}+A_{Te}}$							0.89	0.89	0.51	0.51	1.31	1.31
RBr+RBr@A_{Te}+A_{Te}	-0.14	-0.14	-0.07	-0.07	-0.07	-0.07	0.89	0.89	0.53	0.53	1.33	1.33
RBr+RI@A_{Te}+A_{Te}	-0.14	-0.19	-0.07	0.00	-0.08	0.05	0.90	0.90	0.52	0.52	1.33	1.33
RI+RI@A_{Te}+A_{Te}	-0.17	-0.17	-0.01	-0.01	0.05	0.05	0.90	0.90	0.52	0.52	1.32	1.32
C_9H_{20}@A_{Te}+A_{Te}							0.89	0.89	0.53	0.53	1.32	1.32
RBr (C_4H_9Br)	-0.16		-0.10		-0.03							
RI (C_4H_9I)	-0.06		-0.08		0.08							
C_9H_{20}												

Table 2S Dipole moments μ(Debye), dipole electric field isotropic and anisotropic electric field polarizabilities (au) of $\mathbf{A_x+A_x}$, $\mathbf{RX+RX'@A_x+A_x}$, $\mathbf{A'_x+A'_x}$, and $\mathbf{RX+RX'@A'_x+A'_x}$, at M06-2X/6-31G(d,p) level of theory.

		$\mathbf{A_x+A_x}$,			$\mathbf{A'_x+A'_x}$,			% (A-A')	
	μ	iso	aniso	% $_{iso-aniso}$	iso	aniso	% $_{iso-aniso}$	iso	aniso
$\mathbf{A_{Se}+A_{Se}}$	0.0015	1521.34	1008.03	33.7	1816.44	1242.05	57.0	16.2	18.8
$\mathbf{RBr+RBr@A_{Se}+A_{Se}}$	1.4506	1590.86	1023.25	35.7	1881.93	1262.12	60.6	15.5	18.9
$\mathbf{RBr+RI@A_{Se}+A_{Se}}$	1.3307	1588.64	1029.83	35.2	1871.08	1275.48	57.8	15.1	19.3
$\mathbf{RI+RI@A_{Se}+A_{Se}}$	1.1175	1597.64	1027.44	35.7	1895.49	1241.17	63.7	15.7	17.2
$\mathbf{C_9H_{20}@A_{Se}+A_{Se}}$	0.2671	1576.74	1029.73	34.7	1886.02	1286.84	58.2	16.4	20.0
$\mathbf{A_{Se}+A_{Te}}$	8.0431	1585.30	1071.63	32.4	1870.11	1333.24	50.1	15.2	19.6
$\mathbf{RBr+RBr@A_{Se}+A_{Te}}$	7.8370	1655.81	1083.37	34.6	1954.84	1313.41	59.2	15.3	17.5
$\mathbf{RI+RBr@A_{Se}+A_{Te}}$	7.7264	1665.75	1085.47	34.8	1963.57	1320.26	59.3	15.2	17.8
$\mathbf{RBr+RI@A_{Se}+A_{Te}}$	8.1691	1666.64	1084.94	34.9	1966.97	1310.94	60.5	15.3	17.2
$\mathbf{RI+RI@A_{Se}+A_{Te}}$	7.5407	1681.06	1102.56	34.4	1973.74	1332.58	58.2	14.8	17.3
$\mathbf{C_9H_{20}@A_{Se}+A_{Te}}$	7.8024	1641.21	1086.36	33.8	1932.94	1354.50	53.2	15.1	19.8
$\mathbf{A_{Te}+A_{Te}}$	0.0059	1669.60	1121.13	32.9	1980.1	1358.75	55.4	15.7	17.5
$\mathbf{RBr+RBr@A_{Te}+A_{Te}}$	0.5578	1735.83	1138.6	34.4	2039.62	1379.18	58.0	14.9	17.4
$\mathbf{RBr+RI@A_{Te}+A_{Te}}$	0.5204	1748.09	1165.26	33.3	2049.52	1409.12	55.0	14.7	17.3
$\mathbf{RI+RI@A_{Te}+A_{Te}}$	0.3940	1758.40	1166.58	33.7	2060.07	1396.57	56.9	14.6	16.5
$\mathbf{C_9H_{20}@A_{Te}+A_{Te}}$	0.1600	1719.59	1135.14	34.0	2041.26	1401.95	56.3	15.8	19.0
RBr (C_4H_9Br)	2.3601	60.6347	27.7507						
RI (C_4H_9I)	2.3272	67.0546	45.0807						
$\mathbf{C_9H_{20}}$	0.0476	100.966	37.8254						

Table 3S. ^{1}H NMR shifts of 1-C_4H_9Br and 1-C_4H_9I inside capsules $\mathbf{A_Y+A_{Y'}}$, Y, Y′=Se and Te.

^{1}H NMR shifts of 1-C_4H_9Br

	$\mathbf{A_{Se}+A_{Se}}$			$\mathbf{A_{Se}+A_{Te}}$				$\mathbf{A_{Te}+A_{Te}}$		
RBr	**RBr + RBr**		**RBr + RI**	**RBr + RBr**		**RBr+RI**		**RBr + RBr**		**RBr + RI**
3.20	-0.81	-0.92	-0.74	-0.98	-0.16	-0.99	0.21	-0.44	-0.37	0.54
3.20	-0.44	-0.38	-0.42	-0.13	-0.08	-0.09	-0.23	0.51	0.50	0.38
1.73	-2.35	-2.36	-2.25	-2.42	-1.94	-2.42	-1.93	-2.06	-2.02	-1.89
1.73	-2.23	-2.25	-2.04	-2.18	-1.88	-2.00	-2.03	-1.73	-1.81	-1.52
1.22	-2.48	-2.87	-2.94	-2.50	-2.65	-3.02	-2.78	-2.34	-2.74	-2.55
1.22	-2.87	-2.47	-2.50	-2.90	-2.31	-2.63	-2.39	-2.78	-2.32	-2.69
1.12	-3.67	-3.10	-2.83	-3.78	-2.80	-2.80	-2.64	-3.65	-2.86	-3.35
0.91	-3.96	-3.66	-3.62	-4.01	-3.49	-3.72	-3.60	-4.06	-3.70	-3.67
0.91	-3.07	-3.91	-4.05	-3.16	-3.90	-4.05	-3.93	-2.74	-3.96	-2.57

^{1}H NMR shifts of 1-C_4H_9I

	$\mathbf{A_{Se}+A_{Se}}$			$\mathbf{A_{Se}+A_{Te}}$				$\mathbf{A_{Te}+A_{Te}}$		
RI	**RI + RI**		**RBr + RI**	**RI + RI**		**RBr+RI**		**RI + RI**		**RBr + RI**
2.72	-1.35	-1.59	-1.69	-0.82	-0.83	-1.31	-1.22	-0.21	-0.38	-0.42
2.72	-1.07	-0.89	-0.98	-0.74	-0.17	-0.55	-1.02	-0.43	0.11	-0.19
1.67	-2.29	-2.31	-2.34	-2.05	-1.90	-1.95	-2.32	-1.84	-1.77	-1.68
1.67	-2.21	-2.14	-2.31	-2.23	-1.81	-1.99	-2.25	-1.32	-1.62	-1.83
1.23	-2.40	-2.86	-2.44	-2.98	-2.38	-2.44	-2.57	-2.47	-2.54	-2.66
1.23	-2.87	-2.44	-2.86	-2.73	-2.51	-2.51	-3.07	-2.59	-2.53	-2.60
0.89	-3.75	-2.76	-3.79	-4.02	-2.54	-3.50	-3.85	-3.63	-2.68	-2.34
0.89	-4.05	-3.71	-4.05	-3.68	-3.32	-3.77	-4.26	-3.61	-3.31	-3.74
1.10	-2.91	-4.09	-3.04	-2.66	-3.74	-2.71	-2.87	-2.45	-4.16	-4.15

Table 4S. ^{1}H NMR shifts of 1-C_4H_9Br and 1-C_4H_9I inside capsules $\mathbf{A'_Y+A'_{Y'}}$, Y, Y′=Se and Te.

^{1}H NMR shifts of 1-C_4H_9Br

	$\mathbf{A'_{Se}+A'_{Se}}$			$\mathbf{A'_{Se}+A'_{Te}}$				$\mathbf{A'_{Te}+A'_{Te}}$		
RBr	**RBr + RBr**		**RBr + RI**	**RBr + RBr**		**RBr + RI**		**RBr + RBr**		**RBr + RI**
3.20	-0.90	-0.99	-0.83	-1.06	-0.25	-1.08	0.12	-0.51	-0.43	0.44
3.20	-0.51	-0.45	-0.52	-0.22	-0.16	-0.17	-0.32	0.45	0.44	0.28
1.73	-2.44	-2.45	-2.36	-2.51	-2.06	-2.53	-2.03	-2.14	-2.09	-1.99
1.73	-2.30	-2.33	-2.16	-2.28	-1.96	-2.09	-2.12	-1.80	-1.87	-1.63
1.22	-2.56	-2.95	-3.04	-2.59	-2.79	-3.15	-2.90	-2.42	-2.83	-2.65
1.22	-2.98	-2.55	-2.60	-3.01	-2.39	-2.73	-2.49	-2.88	-2.39	-2.78
0.91	-3.76	-3.76	-3.74	-3.89	-3.49	-3.82	-3.71	-3.73	-3.78	-3.51
0.91	-4.08	-4.03	-4.16	-4.15	-4.09	-4.18	-4.08	-4.16	-4.07	-3.80
1.12	-3.23	-3.20	-2.95	-3.33	-2.91	-2.98	-2.83	-2.88	-2.99	-2.75

^{1}H NMR shifts of 1-C_4H_9I

	$\mathbf{A'_{Se}+A'_{Se}}$			$\mathbf{A'_{Se}+A'_{Te}}$				$\mathbf{A'_{Te}+A'_{Te}}$		
RI	**RI + RI**		**RBr + RI**	**RI + RI**		**RBr + RI**		**RI + RI**		**RBr + RI**
2.72	-1.42	-1.66	-1.78	-0.91	-0.93	-1.37	-1.32	-0.33	-0.48	-0.52
2.72	-1.14	-0.95	-1.08	-0.83	-0.31	-0.61	-1.11	-0.53	0.02	-0.29
1.67	-2.38	-2.39	-2.43	-2.17	-2.03	-2.01	-2.42	-1.99	-1.87	-1.75
1.67	-2.29	-2.22	-2.41	-2.35	-1.97	-2.05	-2.35	-1.45	-1.71	-1.92
1.23	-2.48	-2.95	-2.54	-3.12	-2.53	-2.53	-2.68	-2.61	-2.66	-2.76
1.23	-2.97	-2.53	-2.95	-2.88	-2.68	-2.61	-3.20	-2.73	-2.65	-2.73
0.89	-3.85	-3.82	-3.85	-4.19	-3.54	-3.59	-3.97	-3.80	-3.46	-3.85
0.89	-4.17	-4.21	-4.09	-3.85	-3.95	-3.86	-4.40	-3.81	-4.29	-4.25
1.10	-3.06	-2.92	-3.17	-2.87	-2.78	-2.85	-3.06	-2.68	-2.87	-2.53

Table 5S. ^{1}H NMR shifts of C_9H_{20} inside capsules, in solvent and experimental values.

$A_{Se}+A_{Se}$	$A_{Se}+A_{Te}$	$A_{Te}+A_{Te}$	$A'_{Se}+A'_{Se}$	$A'_{Se}+A'_{Te}$	$A'_{Te}+A'_{Te}$	free	expt
-3.86	-3.23	-3.34	-5.01	-3.37	-4.3	1.14	0.88
-3.25	-3.54	-3.69	-4.31	-3.66	-4.53	0.94	0.88
-3.60	-3.73	-3.54	-4.54	-3.89	-4.59	0.94	0.88
-1.74	-2.52	-2.09	-2.75	-2.60	-3.39	1.38	1.31
-2.89	-2.66	-2.39	-3.75	-2.77	-3.51	1.38	1.31
-3.05	-2.93	-2.33	-3.7	-3.05	-3.34	1.34	1.29
-3.04	-2.80	-1.90	-3.84	-2.90	-3.29	1.34	1.29
-3.54	-2.58	-2.24	-3.86	-2.66	-3.17	1.36	1.29
-2.32	-3.53	-2.23	-2.91	-3.60	-2.93	1.36	1.29
-3.11	-2.65	-1.78	-3.57	-2.76	-2.8	1.37	1.29
-2.81	-2.56	-1.56	-3.27	-2.66	-2.7	1.37	1.29
-3.68	-2.06	-2.24	-4.16	-2.13	-3.02	1.36	1.29
-2.75	-2.91	-1.72	-3.4	-3.01	-2.99	1.36	1.29
-2.97	-2.59	-2.50	-3.67	-2.69	-3.34	1.34	1.29
-3.05	-2.65	-2.16	-3.79	-2.76	-3.36	1.34	1.29
-2.34	-1.41	-1.80	-3.51	-1.52	-3.42	1.39	1.31
-2.50	-2.49	-2.13	-3.51	-2.61	-3.44	1.39	1.31
-3.26	-3.38	-3.42	-4.63	-3.88	-4.44	0.94	0.88
-3.65	-3.01	-3.13	-4.62	-3.53	-4.52	0.94	0.88
-3.36	-3.71	-3.49	-4.31	-3.17	-4.29	1.14	0.88

Table 6S. Average of ^{1}H NMR shifts of C_9H_{20} for each C atom inside capsules, in solvent and experimental values.

$A_{Se}+A_{Se}$	$A_{Se}+A_{Te}$	$A_{Te}+A_{Te}$	$A'_{Se}+A'_{Se}$	$A'_{Se}+A'_{Te}$	$A'_{Te}+A'_{Te}$	free	expt
-3.57	-3.50	-3.52	-4.62	-3.64	-4.47	1.01	0.88
-2.31	-2.59	-2.24	-3.25	-2.69	-3.45	1.38	1.31
-3.04	-2.87	-2.12	-3.77	-2.97	-3.32	1.34	1.29
-2.93	-3.06	-2.23	-3.39	-3.13	-3.05	1.36	1.29
-2.96	-2.61	-1.67	-3.42	-2.71	-2.75	1.37	1.29
-3.22	-2.49	-1.98	-3.78	-2.57	-3.01	1.36	1.29
-3.01	-2.62	-2.33	-3.73	-2.73	-3.35	1.34	1.29
-2.42	-1.95	-1.97	-3.51	-2.06	-3.43	1.39	1.31
-3.42	-3.37	-3.35	-4.52	-3.53	-4.42	1.01	0.88

Table 7S. BSSE corrected ΔE (eV), deformation energy(Def), 2-body(2B), 3-body(3B) terms in eV at M06-2X/6-31G(d.p).

	ΔE_u[a]	ΔE_{bsse}	Def.[b]	$2B_1$[c]	$2B_2$[d]	$2B_3$[e]	3B	def1[f]	def2[g]	def3[h]	def4[i]
$2C_4H_9Br$	-0.32	-0.23	0.01	-0.24							
$C_4H_9Br+C_4H_9I$	-0.29	-0.22	0.01	-0.23							
$2C_4H_9I$	-0.25	-0.22	0.01	-0.23							
$A_{Se}+A_{Se}$	-3.95	-1.80	0.72	-2.51							
$A_{Se}+A_{Te}$	-3.91	-2.77	1.17	-3.94							
$A_{Te}+A_{Te}$	-5.88	-4.60	2.23	-6.84							
$A'_{Te}+A'_{Te}$	-5.72	-4.58	2.24	-6.82							
	RX+RX′ & A_Y+A_Y'			OR	C_9H_{20}	**& A_Y+A_Y'**					
RBr+RBr@$A_{Se}+A_{Se}$	-2.81	-0.87	0.33	-1.19				0.00	0.33		
RBr+RI@$A_{Se}+A_{Se}$	-1.67	-0.97	0.26	-1.23				0.01	0.25		
RI+RI@$A_{Se}+A_{Se}$	-1.74	-1.05	0.23	-1.28				0.01	0.22		
C_9H_{20}@$A_{Se}+A_{Se}$	-2.00	-0.94	0.01	-0.95				0.00	0.01		
RBr+RBr@$A_{Se}+A_{Se}$	-1.65	-0.98	0.29	-1.27				0.01	0.29		
RBr+RI@$A_{Se}+A_{Se}$	-1.67	-0.98	0.32	-1.30				0.03	0.26		
RI+RBr@$A_{Se}+A_{Te}$	-1.66	-1.00	0.37	-1.37				0.01	0.31		
RI+RI@$A_{Se}+A_{Te}$	-1.61	-0.93	0.38	-1.31				0.16	0.21		
C_9H_{20}@$A_{Se}+A_{Te}$	-1.27	-0.83	0.14	-0.97				0.03	0.11		
RBr+RBr@$A_{Te}+A_{Te}$	-1.46	-0.83	0.50	-1.33				0.06	0.33		
RBr+RI@$A_{Te}+A_{Te}$	-1.47	-0.89	0.50	-1.39				0.19	0.31		
RI+RI@$A_{Te}+A_{Te}$	-2.81	-0.87	0.32	-1.19				0.24	0.26		
C_9H_{20}@$A_{Te}+A_{Te}$	-1.25	-0.85	0.17	-1.01				0.05	0.12		
			RX & RX′ & A_Y+A_Y'								
RBr+RBr@$A_{Se}+A_{Se}$	-3.34	-1.19	0.10	-0.35	-0.34	-0.08	-0.52	0.00	0.05	0.05	
RBr+RI@$A_{Se}+A_{Se}$	-1.95	-1.22	0.08	-0.41	-0.25	-0.06	-0.57	0.01	0.03	0.04	
RI+RI@$A_{Se}+A_{Se}$	-1.98	-1.28	0.05	-0.32	-0.31	-0.06	-0.65	0.01	0.02	0.02	
RBr+RBr@$A_{Se}+A_{Se}$	-1.90	-1.17	0.10	-0.34	-0.42	-0.06	-0.44	0.01	0.04	0.05	
RBr+RI@$A_{Se}+A_{Se}$	-1.93	-1.23	0.10	-0.48	-0.26	-0.06	-0.53	0.03	0.03	0.04	
RI+RBr@$A_{Se}+A_{Te}$	-1.95	-1.24	0.07	-0.43	-0.34	0.00	-0.53	0.01	0.02	0.04	
RI+RI@$A_{Se}+A_{Te}$	-1.90	-1.23	0.22	-0.34	-0.39	-0.08	-0.63	0.16	0.03	0.03	
RBr+RBr@$A_{Te}+A_{Te}$	-1.93	-1.19	0.15	-0.45	-0.46	-0.03	-0.40	0.06	0.05	0.05	
RBr+RI@$A_{Te}+A_{Te}$	-1.74	-1.08	0.32	-0.36	-0.52	-0.07	-0.45	0.19	0.06	0.07	
RI+RI@$A_{Te}+A_{Te}$	-1.72	-1.12	0.34	-0.43	-0.44	-0.07	-0.52	0.24	0.05	0.05	
	RX & RX′ & A_Y & A_Y'			OR	C_9H_{20}	**& A_Y & A_Y'**					
RBr+RBr@$A_{Se}+A_{Se}$	-7.29	-2.96	0.71					0.30	0.30	0.05	0.05
RBr+RI@$A_{Se}+A_{Se}$	-4.70	-2.96	0.64					0.29	0.28	0.03	0.04
RI+RI@$A_{Se}+A_{Se}$	-4.73	-3.03	0.60					0.28	0.28	0.02	0.02
C_9H_{20}@$A_{Se}+A_{Se}$	-5.95	-2.67	0.71					0.34	0.36	0.01	
RBr+RBr@$A_{Se}+A_{Se}$	-5.81	-3.93	1.12					0.46	0.57	0.04	0.05
RBr+RI@$A_{Se}+A_{Se}$	-5.84	-3.98	1.11					0.58	0.46	0.03	0.04
RI+RBr@$A_{Se}+A_{Te}$	-5.86	-4.00	1.06					0.45	0.55	0.02	0.04
RI+RI@$A_{Se}+A_{Te}$	-5.81	-3.97	1.21					0.50	0.64	0.03	0.03
C_9H_{20}@$A_{Se}+A_{Te}$	-5.18	-3.57	1.29					0.53	0.64	0.11	
RBr+RBr@$A_{Te}+A_{Te}$	-7.81	-5.80	2.14					1.02	1.03	0.05	0.05
RBr+RI@$A_{Te}+A_{Te}$	-7.62	-5.68	2.43					1.15	1.15	0.06	0.07
RI+RI@$A_{Te}+A_{Te}$	-7.59	-5.72	2.41					1.15	1.16	0.05	0.05
C_9H_{20}@$A_{Te}+A_{Te}$	-7.12	-5.42	2.42					1.15	1.15	0.12	

[a] Uncorrected BSSE dissociation energy.

[b] Total deformation energy.

[c] 2-Body term with respect to dimer (first group); cage + guests (second group); cage + 1st guests (third group).

[d] 2-Body term with respect to cage + 2nd guest (third group).

[e] 2-Body term with respect to 1st guest +2nd guest (third group).

[f] Deformation energy of the cage (second group); of the cage; of the 1st cavitand (third group).

[g] Deformation energy of the encapsulation dimer or of nonane (second group); of the 1st guest (third group); of the 2nd cavitand (forth group)

[h] Deformation energy of the 2nd guest (third group); of the 1st guest (forth group).

[i] Deformation energy of the 2nd guest (forth group).

Table 8S. HOMO-LUMO molecular orbital gaps in eV.

	$\mathbf{A_{Se}+A_{Se}}$	$\mathbf{A_{Se}+A_{Te}}$	$\mathbf{A_{Te}+A_{Te}}$	$\mathbf{A'_{Se}+A'_{Se}}$	$\mathbf{A'_{Se}+A'_{Te}}$	$\mathbf{A'_{Te}+A'_{Te}}$	$\mathbf{A_{Te}+A_{Te}}$
--	5.568	4.786	4.544	5.642	4.769	4.535	4.544
2RBr	5.476	4.558	4.435	5.482	4.541	4.432	4.435
RBr-RI	5.155	4.543	4.413	5.165	4.536	4.404	4.413
RBr-RI	5.155	4.477	4.413	5.165	4.475	4.404	4.413
2RI	4.892	4.677	4.421	4.9	4.689	4.417	4.421
C_9H_{20}	5.530	4.746	4.487	5.565	4.746	4.482	4.487

Table 9S: Geometries of the minimum calculated structures at M06-2X/LAN2LDZ and 6-31G(d,p) .

M06-2X/6-31G(d,p)

n-C_4H_9Br,

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-0.039738	0.781365	0.000227
2	1	0	-0.040410	1.410996	-0.889571
3	1	0	-0.040612	1.410707	0.890240
4	6	0	1.109529	-0.208305	0.000194
5	6	0	2.462528	0.505762	-0.000266
6	1	0	1.026835	-0.856746	-0.879106
7	1	0	1.027116	-0.856230	0.879908
8	6	0	3.627582	-0.480537	0.000004
9	1	0	2.529526	1.158679	-0.879048
10	1	0	2.529808	1.159131	0.878126
11	1	0	4.589280	0.037859	0.000331
12	1	0	3.591690	-1.125082	0.883313
13	1	0	3.592237	-1.124927	-0.883400
14	35	0	-1.764711	-0.137260	-0.000050

n-C_4H_9I,

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	4.111516	-0.520232	-0.000063
2	6	0	2.969028	0.492489	-0.000051
3	1	0	5.084352	-0.023012	0.000049
4	1	0	4.061715	-1.163581	0.883405
5	1	0	4.061902	-1.163477	-0.883598
6	6	0	1.599149	-0.191584	0.000150
7	1	0	3.050160	1.143801	0.878561
8	1	0	3.049871	1.143690	-0.878777
9	1	0	1.508375	-0.838949	-0.879177
10	1	0	1.508324	-0.838490	0.879818
11	6	0	0.477651	0.832376	0.000022
12	1	0	0.496247	1.463223	-0.888648
13	1	0	0.496211	1.463152	0.888758
14	53	0	-1.476627	-0.091786	-0.000014

M06-2X/LAN2LDZ

n-C_4H_9Br,

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-0.008154	0.799984	0.000006
2	1	0	-0.011894	1.423804	-0.894477
3	1	0	-0.012005	1.423995	0.894354
4	6	0	1.137084	-0.206588	0.000279
5	6	0	2.501695	0.510506	-0.000020
6	1	0	1.059998	-0.854067	-0.881330
7	1	0	1.060068	-0.853484	0.882337
8	6	0	3.664533	-0.495191	-0.000137
9	1	0	2.574520	1.160997	-0.881428
10	1	0	2.574902	1.161011	0.881332
11	1	0	4.632969	0.014798	0.000377
12	1	0	3.619997	-1.139321	0.885163
13	1	0	3.620573	-1.138573	-0.885974
14	35	0	-1.796859	-0.138612	-0.000032

n-C_4H_9I,

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	0.487499	0.847688	0.000201
2	1	0	0.505960	1.474879	-0.892524
3	1	0	0.505782	1.474756	0.893016
4	6	0	1.611852	-0.187112	0.000269
5	6	0	2.992846	0.498964	-0.000249
6	1	0	1.523035	-0.834143	-0.880905
7	1	0	1.523322	-0.833514	0.881931
8	6	0	4.133014	-0.532454	-0.000024
9	1	0	3.079016	1.147395	-0.881917
10	1	0	3.079402	1.148117	0.880840
11	1	0	5.112650	-0.044217	-0.000095
12	1	0	4.074523	-1.174931	0.885708
13	1	0	4.074575	-1.175290	-0.885491
14	53	0	-1.487350	-0.093313	-0.000033

A_{Se}+A_{Se}

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	34	0	0.062546	3.452699	-3.477167
2	8	0	-6.129327	2.408324	-4.345238
3	34	0	0.061919	-3.477444	-3.451422
4	7	0	-1.264002	4.357357	-2.530342
5	8	0	-6.129276	-2.436694	-4.328410
6	34	0	0.063164	3.477823	3.451703
7	7	0	-1.264514	2.500182	-4.375068
8	34	0	0.062604	-3.451871	3.476450
9	8	0	-6.128773	4.329822	-2.436581

10	7	0	-1.264521	-2.529551	-4.355037
11	8	0	-6.130008	-4.346494	-2.408238
12	7	0	-1.265160	-4.376941	-2.500332
13	6	0	-9.911767	2.544824	-2.560512
14	1	0	-10.294935	3.535060	-2.295319
15	8	0	-6.129085	-2.408460	4.347025
16	7	0	-1.263256	2.529816	4.355303
17	6	0	-8.373130	2.565376	-2.581588
18	1	0	-8.052507	3.301879	-3.323061
19	8	0	-6.127949	2.436520	4.329113
20	7	0	-1.264116	4.377118	2.500663
21	6	0	-7.778917	1.224800	-3.011276
22	8	0	-6.128919	4.346290	2.408532
23	6	0	-6.653217	1.188906	-3.849554
24	7	0	-1.264313	-2.500948	4.376311
25	6	0	-6.097261	-0.014042	-4.282396
26	1	0	-5.274089	-0.016563	-4.986109
27	7	0	-1.264009	-4.354741	2.528026
28	8	0	-6.128808	-4.328378	2.436727
29	6	0	-6.653210	-1.213932	-3.841251
30	6	0	-7.779184	-1.244114	-3.003108
31	6	0	-8.315828	-0.008271	-2.604963
32	1	0	-9.192197	-0.006195	-1.963295
33	6	0	-7.778343	3.003813	-1.244067
34	6	0	-8.314775	2.605365	-0.008238
35	1	0	-9.190896	1.963361	-0.006196
36	6	0	-7.778046	3.011803	1.224849
37	6	0	-6.652669	3.850534	1.189018
38	6	0	-6.096812	4.283531	-0.013933
39	1	0	-5.273784	4.987431	-0.016451
40	6	0	-6.652615	3.842281	-1.213881
41	6	0	-4.876460	3.878295	-2.867180
42	6	0	-3.717231	4.431695	-2.408203
43	1	0	-3.717490	5.240557	-1.688533
44	6	0	-2.464387	3.945996	-2.927879
45	6	0	-2.464703	2.900935	-3.966120
46	6	0	-7.778954	-3.003390	1.244343
47	6	0	-3.717934	2.378667	-4.447990
48	1	0	-3.718796	1.653745	-5.252164
49	6	0	-8.373800	-2.581813	-2.564912
50	1	0	-8.053262	-3.323056	-3.301687
51	6	0	-9.912431	-2.560842	-2.544024
52	1	0	-10.295782	-3.549993	-2.275075
53	6	0	-8.315857	-2.605357	0.008614
54	1	0	-9.192175	-1.963620	0.006689
55	6	0	-7.779265	-3.011810	-1.224581
56	6	0	-6.653729	-3.850305	-1.188866
57	6	0	-6.097459	-4.282954	0.014036
58	1	0	-5.274335	-4.986723	0.016382
59	6	0	-6.652983	-3.841541	1.213994
60	6	0	-8.373073	-2.565021	2.582183
61	1	0	-8.052513	-3.301830	3.323371
62	6	0	-4.877388	-3.898236	-2.841423
63	6	0	-4.876963	-2.867236	-3.876968
64	6	0	-3.717650	-2.407400	-4.429491
65	1	0	-3.717705	-1.686905	-5.237612
66	6	0	-2.464896	-2.927577	-3.944174
67	6	0	-2.465288	-3.967257	-2.900545
68	6	0	-3.718608	-4.449682	-2.378954
69	1	0	-3.719614	-5.254647	-1.654912
70	6	0	-6.652703	-1.189093	3.850652
71	6	0	-7.778167	-1.224794	3.012034
72	6	0	-8.314591	0.008380	2.605372
73	1	0	-9.190746	0.006419	1.963413
74	6	0	-7.777844	1.244141	3.003524
75	6	0	-6.651984	1.213825	3.841823
76	6	0	-6.096436	0.013847	4.283237
77	1	0	-5.273302	0.016245	4.987019
78	6	0	-4.876288	3.898214	2.841822
79	6	0	-4.875770	2.867300	3.877464
80	6	0	-3.716416	2.407621	4.430032
81	1	0	-3.716466	1.687066	5.238101
82	6	0	-2.463687	2.927822	3.944637
83	6	0	-2.464190	3.967482	2.900968
84	6	0	-3.717557	4.449735	2.379338
85	1	0	-3.718655	5.254593	1.655173
86	6	0	-8.372376	2.581829	2.565264
87	1	0	-8.051737	3.323083	3.301975
88	6	0	-9.911025	2.560985	2.544549
89	1	0	-10.320569	1.841578	1.827728
90	1	0	-10.294339	2.295651	3.534690
91	6	0	-2.464328	-3.944176	2.926604
92	6	0	-2.464516	-2.901173	3.966945
93	6	0	-3.717711	-2.379813	4.449962
94	1	0	-3.718553	-1.656029	5.255167
95	6	0	-4.876614	-2.841903	3.898483
96	6	0	-4.876420	-3.876992	2.867018
97	6	0	-3.717222	-4.429251	2.406554
98	1	0	-3.717481	-5.237026	1.685672
99	6	0	-9.911706	-2.543744	2.561703
100	1	0	-10.294659	-2.274379	3.550893
101	1	0	-10.321164	-1.826927	1.842243
102	6	0	-4.876773	2.841678	-3.897135
103	34	0	-0.063348	-4.900221	0.017704
104	8	0	6.128522	-4.786783	-1.336049
105	34	0	-0.063675	-0.017754	-4.897978
106	7	0	1.263238	-4.859174	1.326490
107	8	0	6.127617	-1.373477	-4.774560
108	34	0	-0.061958	0.017615	4.899543
109	7	0	1.263653	-4.872661	-1.291068
110	34	0	-0.061594	4.901453	-0.017795
111	8	0	6.128091	-4.774336	1.372348
112	7	0	1.262848	-1.326699	-4.858495
113	8	0	6.128442	1.335055	-4.785830
114	7	0	1.263564	1.290868	-4.869832
115	6	0	9.911328	-3.611052	0.013805
116	1	0	10.320809	-2.595483	0.009477
117	1	0	10.294815	-4.118166	0.904592
118	8	0	6.130436	4.785291	1.334713
119	7	0	1.264529	1.326433	4.858153
120	6	0	8.372694	-3.640319	0.014142
121	1	0	8.051987	-4.685355	0.018580

122	8	0	6.129330	1.372562	4.773843
123	7	0	1.265008	-1.291174	4.872223
124	6	0	7.778111	-3.005644	-1.242356
125	8	0	6.129853	-1.335765	4.785652
126	6	0	6.652484	-3.577648	-1.856352
127	7	0	1.265552	4.872477	1.290810
128	6	0	6.096323	-3.041520	-3.016884
129	1	0	5.272974	-3.540980	-3.512318
130	7	0	1.264742	4.860835	-1.326838
131	8	0	6.129453	4.774609	-1.373677
132	6	0	6.651927	-1.884857	-3.561844
133	6	0	7.777833	-1.266560	-2.995005
134	6	0	8.314664	-1.850437	-1.835389
135	1	0	9.190619	-1.394427	-1.383083
136	6	0	7.778622	-2.995216	1.265476
137	6	0	8.315863	-1.835817	1.849446
138	1	0	9.192106	-1.383869	1.393642
139	6	0	7.779293	-1.242545	3.004531
140	6	0	6.653476	-1.856250	3.576472
141	6	0	6.096983	-3.016598	3.040336
142	1	0	5.273552	-3.511877	3.539806
143	6	0	6.652490	-3.561676	1.883700
144	6	0	4.875747	-4.763945	0.748594
145	6	0	3.716482	-4.824423	1.465008
146	1	0	3.716613	-4.878269	2.546348
147	6	0	2.463636	-4.854144	0.754402
148	6	0	2.463895	-4.861715	-0.718651
149	6	0	3.717099	-4.839086	-1.428935
150	1	0	3.717796	-4.904187	-2.509640
151	6	0	8.372327	-0.015352	-3.639933
152	1	0	8.051609	-0.019530	-4.684965
153	6	0	9.910959	-0.015623	-3.610690
154	1	0	10.294427	0.871033	-4.124981
155	1	0	10.320471	-0.011666	-2.595129
156	6	0	8.315255	1.834310	-1.850127
157	1	0	9.191185	1.381816	-1.394262
158	6	0	7.778253	1.241292	-3.005101
159	6	0	6.652625	1.855500	-3.576901
160	6	0	6.097003	3.016314	-3.040909
161	1	0	5.273688	3.511967	-3.540225
162	6	0	6.653160	3.561379	-1.884545
163	6	0	8.373943	3.638945	-0.015238
164	1	0	8.053610	4.684095	-0.019352
165	6	0	4.875871	0.711885	-4.770128
166	6	0	4.875426	-0.749393	-4.763950
167	6	0	3.716062	-1.465601	-4.824788
168	1	0	3.716065	-2.546902	-4.879363
169	6	0	2.463285	-0.754798	-4.853649
170	6	0	2.463697	0.718273	-4.859916
171	6	0	3.717025	1.428356	-4.837161
172	1	0	3.717841	2.509110	-4.901444
173	6	0	6.654130	3.576298	1.855418
174	6	0	7.779765	3.004240	1.241445
175	6	0	8.316369	1.849116	1.834538
176	1	0	9.192330	1.393105	1.382242
177	6	0	7.779493	1.265273	2.994201
178	6	0	6.653652	1.883689	3.561009
179	6	0	6.098020	3.040344	3.016008
180	1	0	5.274749	3.539835	3.511524
181	6	0	4.877302	-0.712555	4.770424
182	6	0	4.877019	0.748694	4.763447
183	6	0	3.717744	1.465092	4.823860
184	1	0	3.717849	2.546420	4.877756
185	6	0	2.464915	0.754406	4.853507
186	6	0	2.465194	-0.718691	4.861180
187	6	0	3.718436	-1.428894	4.838393
188	1	0	3.719164	-2.509606	4.903378
189	6	0	8.373861	0.013989	3.639184
190	1	0	8.053319	0.018404	4.684272
191	6	0	2.465186	4.855531	-0.754942
192	6	0	2.465657	4.861818	0.718171
193	6	0	3.718972	4.838191	1.428268
194	1	0	3.719783	4.902429	2.509021
195	6	0	4.877768	4.770492	0.711781
196	6	0	4.877285	4.764565	-0.749494
197	6	0	3.717981	4.826141	-1.465712
198	1	0	3.718106	4.880848	-2.547011
199	6	0	9.912559	3.609147	-0.015777
200	1	0	10.321718	2.593448	-0.011806
201	1	0	10.295697	4.116243	-0.906720
202	6	0	7.778924	2.994238	-1.266325
203	6	0	4.876029	-4.771146	-0.712665
204	6	0	9.912479	0.013890	3.609675
205	1	0	10.321824	0.009706	2.594050
206	1	0	10.295895	0.904697	4.116797
207	1	0	-10.321829	-1.841476	-1.827077
208	1	0	-10.295846	-2.295367	-3.534090
209	1	0	-10.294310	3.550147	2.275541
210	1	0	-10.295455	-3.533802	2.296676
211	1	0	-10.321292	1.828201	-1.840897
212	1	0	-10.295234	2.275664	-3.549563
213	1	0	10.294463	-4.125499	-0.872902
214	1	0	10.294066	-0.906467	-4.117988
215	1	0	10.296363	4.123371	0.870775
216	1	0	10.295828	-0.872793	4.124010

$A_{Se}+A_{Te}$

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.305689	2.020659	3.026874
2	6	0	-7.710763	0.622636	3.190807
3	6	0	-7.710557	2.708123	1.798691
4	1	0	-7.986328	2.601217	3.896310
5	6	0	-8.247912	-0.509361	2.555163
6	6	0	-6.584772	0.425708	4.005919
7	6	0	-8.247344	2.555958	0.509287
8	6	0	-6.584666	3.536264	1.930219
9	6	0	-7.711168	-1.798787	2.707419

10	6	0	-6.029063	-0.837988	4.199569
11	8	0	-6.060051	1.526881	4.727066
12	6	0	-7.710234	3.191630	-0.622713
13	6	0	-6.028545	4.200381	0.837946
14	8	0	-6.060221	3.779112	3.224034
15	6	0	-8.306203	-3.027009	2.019918
16	6	0	-6.585260	-1.930265	3.535555
17	1	0	-5.206911	-0.976197	4.890949
18	6	0	-4.808825	2.038525	4.370232
19	6	0	-8.305268	3.027640	-2.020702
20	6	0	-6.584237	4.006755	-0.425785
21	1	0	-5.206461	4.891832	0.976168
22	6	0	-4.808888	3.253539	3.559531
23	1	0	-7.986934	-3.896423	2.600558
24	6	0	-7.711000	-3.191012	0.622013
25	8	0	-6.060825	-3.224002	3.778573
26	6	0	-7.710364	1.799291	-2.708041
27	1	0	-7.985763	3.896918	-2.601419
28	8	0	-6.059449	4.727946	-1.526938
29	6	0	-8.247863	-2.555323	-0.510093
30	6	0	-6.585023	-4.006200	0.425315
31	6	0	-4.809474	-3.559479	3.253101
32	6	0	-2.397319	2.088072	4.452855
33	6	0	-8.247442	0.509991	-2.555971
34	6	0	-6.584300	1.930604	-3.535965
35	6	0	-4.808240	4.370977	-2.038601
36	6	0	-2.397403	3.311340	3.636697
37	6	0	-7.710831	-2.707550	-1.799403
38	6	0	-6.029069	-4.199870	-0.838275
39	8	0	-6.060518	-4.727328	1.526602
40	6	0	-4.809323	-4.370523	2.038345
41	6	0	-7.710380	-0.622086	-3.191548
42	6	0	-6.028221	0.838271	-4.199984
43	8	0	-6.059730	3.224341	-3.778781
44	6	0	-4.808373	3.559784	-3.253294
45	6	0	-8.305580	-2.020007	-3.027746
46	6	0	-6.584947	-3.535743	-1.930652
47	1	0	-5.206967	-4.891334	-0.976333
48	6	0	-2.397995	-3.636451	3.311007
49	6	0	-6.584208	-0.425334	-4.006460
50	1	0	-5.205976	0.976372	-4.891273
51	6	0	-2.396723	4.453478	-2.088324
52	1	0	-7.986074	-2.600637	-3.897082
53	8	0	-6.060211	-3.778700	-3.224298
54	6	0	-2.397839	-4.453302	2.088237
55	8	0	-6.059545	-1.526607	-4.727482
56	6	0	-2.396872	3.636572	-3.311126
57	6	0	-4.808769	-3.253219	-3.559487
58	6	0	-4.808437	-2.038329	-4.370367
59	6	0	-2.397258	-3.311149	-3.635937
60	6	0	-2.396947	-2.088139	-4.452521
61	6	0	-3.649429	-4.824693	1.480395
62	6	0	-3.649794	-3.217660	3.886637
63	6	0	-3.648964	1.480239	4.824101
64	6	0	-3.649161	3.887164	3.218046
65	6	0	-3.649174	-3.886827	-3.217525
66	6	0	-3.648455	-1.480279	-4.824163
67	6	0	-3.648333	4.825099	-1.480630
68	6	0	-3.648697	3.217829	-3.886750
69	1	0	-3.653524	-5.481811	0.619378
70	1	0	-3.654255	-2.674378	4.823651
71	1	0	-3.653778	-4.823928	-2.674395
72	1	0	-3.653132	0.618952	5.480867
73	1	0	-3.652391	-0.619237	-5.481248
74	1	0	-3.653564	4.824392	2.675135
75	1	0	-3.652421	5.482332	-0.619703
76	1	0	-3.653172	2.674413	-4.823690
77	7	0	-1.192479	-1.617112	-4.760371
78	7	0	-1.192973	-3.776099	-3.318071
79	7	0	-1.192540	3.318512	-3.775801
80	7	0	-1.192307	4.761285	-1.617123
81	7	0	-1.193024	3.776374	3.319285
82	7	0	-1.192902	1.616660	4.760441
83	7	0	-1.193617	-3.318728	3.775909
84	7	0	-1.193370	-4.761371	1.617214
85	1	0	-9.124526	-1.926536	-0.384616
86	1	0	-9.124595	-0.383710	1.926433
87	1	0	-9.124049	1.927247	0.383658
88	1	0	-9.124306	0.384505	-1.927453
89	6	0	-9.844237	-2.002811	-3.002552
90	1	0	-10.227825	-1.548292	-3.921173
91	1	0	-10.253206	-1.437890	-2.158348
92	6	0	-9.843919	3.002283	-2.003709
93	1	0	-10.252862	2.158112	-1.438718
94	1	0	-10.227572	2.932490	-3.026222
95	6	0	-9.844336	2.003722	3.001236
96	1	0	-10.253156	1.438947	2.156858
97	1	0	-10.227930	3.026269	2.931614
98	6	0	-9.844852	-3.001433	2.002704
99	1	0	-10.253611	-2.157141	1.437764
100	1	0	-10.228629	-2.931707	3.025174
101	1	0	-10.228667	-3.919970	1.548207
102	1	0	-10.228025	-3.025285	-2.932946
103	1	0	-10.227659	3.920927	-1.549369
104	1	0	-10.228252	1.549185	3.919710
105	34	0	0.150094	-4.074755	2.719844
106	34	0	0.151108	4.074459	-2.719661
107	34	0	0.150569	2.719630	4.074527
108	34	0	0.150840	-2.719691	-4.073402
109	6	0	8.373166	-3.570268	-0.711291
110	6	0	7.779754	-3.188273	0.644125
111	6	0	7.779656	-2.697701	-1.816536
112	1	0	8.051462	-4.594877	-0.915579
113	6	0	8.316466	-2.168272	1.447626
114	6	0	6.654103	-3.867450	1.137120
115	6	0	8.316716	-1.447728	-2.167689
116	6	0	6.654162	-3.135939	-2.532654
117	6	0	7.779396	-1.816989	2.697564
118	6	0	6.098601	-3.563411	2.378907
119	8	0	6.126461	-4.951417	0.393903
120	6	0	7.780184	-0.644239	-3.187801
121	6	0	6.099155	-2.379087	-3.563234

122	8	0	6.126597	-4.422068	-2.262259
123	6	0	8.372986	-0.711834	3.570189
124	6	0	6.653769	-2.532916	3.135764
125	1	0	5.273686	-4.146807	2.768380
126	6	0	4.872342	-4.807822	-0.212721
127	6	0	8.373730	0.711159	-3.569674
128	6	0	6.654690	-1.137290	-3.867181
129	1	0	5.274338	-2.768557	-4.146781
130	6	0	4.872355	-4.522276	-1.647119
131	1	0	8.051215	-0.916145	4.594771
132	6	0	7.779770	0.643673	3.188209
133	8	0	6.126236	-2.262489	4.421899
134	6	0	7.780219	1.816440	-2.697148
135	1	0	8.052143	0.915505	-4.594306
136	8	0	6.127062	-0.394084	-4.951165
137	6	0	8.316660	1.447040	2.168197
138	6	0	6.654199	1.136913	3.867351
139	6	0	4.872069	-1.647245	4.522125
140	6	0	2.446989	-4.880064	-0.213328
141	6	0	8.317164	2.167645	-1.447143
142	6	0	6.654746	2.532531	-3.135509
143	6	0	4.872993	0.212599	-4.807433
144	6	0	2.446979	-4.589163	-1.674314
145	6	0	7.779951	2.697145	1.816957
146	6	0	6.099033	2.378862	3.563349
147	8	0	6.126210	0.393742	4.951166
148	6	0	4.872087	-0.212761	4.807217
149	6	0	7.780465	3.187724	-0.643719
150	6	0	6.099607	3.563104	-2.378753
151	8	0	6.127321	2.262060	-4.421670
152	6	0	4.873059	1.647010	-4.521957
153	6	0	8.373754	3.569620	0.711774
154	6	0	6.654465	3.135631	2.532922
155	1	0	5.274188	2.768529	4.146725
156	6	0	2.446708	-1.674329	4.588790
157	6	0	6.654984	3.867063	-1.136889
158	1	0	5.274835	4.146624	-2.768352
159	6	0	2.447642	0.213175	-4.879270
160	1	0	8.052165	4.594269	0.916033
161	8	0	6.127262	4.421905	2.262464
162	6	0	2.446705	-0.213187	4.878740
163	8	0	6.127359	4.951095	-0.393756
164	6	0	2.447686	1.674178	-4.588505
165	6	0	4.873103	4.522419	1.647239
166	6	0	4.873188	4.807687	0.212785
167	6	0	2.447766	4.589613	1.674297
168	6	0	2.447823	4.880080	0.213233
169	6	0	3.712692	0.476527	4.997276
170	6	0	3.712684	-2.356853	4.434578
171	6	0	3.712969	-4.998559	0.476384
172	6	0	3.712991	-4.434515	-2.356724
173	6	0	3.713704	4.435004	2.356814
174	6	0	3.713856	4.998354	-0.476435
175	6	0	3.713598	-0.476543	-4.997897
176	6	0	3.713707	2.356622	-4.434080
177	1	0	3.713094	1.526173	5.264850
178	1	0	3.712841	-3.429057	4.280591
179	1	0	3.713808	4.280851	3.428994
180	1	0	3.713338	-5.266563	1.525916
181	1	0	3.714324	5.266116	-1.526030
182	1	0	3.713184	-4.280173	-3.428879
183	1	0	3.713975	-1.526111	-5.265768
184	1	0	3.713882	3.428776	-4.279729
185	7	0	1.268299	4.991379	-0.374551
186	7	0	1.268284	4.467562	2.260065
187	7	0	1.268216	2.259904	-4.465923
188	7	0	1.268089	-0.374552	-4.990440
189	7	0	1.267503	-4.466552	-2.260016
190	7	0	1.267484	-4.991437	0.374463
191	7	0	1.267232	-2.260123	4.466498
192	7	0	1.267155	0.374760	4.989147
193	1	0	9.192101	1.089911	1.633447
194	1	0	9.191986	-1.633502	1.090721
195	1	0	9.192127	-1.090800	-1.632752
196	1	0	9.192563	1.632755	-1.090105
197	6	0	9.912437	3.541260	0.706306
198	1	0	10.295924	4.215311	-0.066007
199	1	0	10.321543	2.544921	0.508491
200	6	0	9.912409	0.705406	-3.541369
201	1	0	10.321521	0.507585	-2.545031
202	1	0	10.295850	1.676723	-3.869034
203	6	0	9.911850	-3.542136	-0.705673
204	1	0	10.321091	-2.545842	-0.507904
205	1	0	10.295175	-3.869867	-1.677013
206	6	0	9.911672	-0.706337	3.542127
207	1	0	10.320975	-0.508453	2.545880
208	1	0	10.294899	-1.677758	3.869732
209	52	0	-0.254736	-0.950266	4.765466
210	52	0	-0.254479	-4.766431	-0.950318
211	52	0	-0.253679	4.766178	0.950140
212	52	0	-0.253857	0.950270	-4.765518
213	1	0	10.294991	0.065951	4.216300
214	1	0	10.295138	-4.216176	0.066747
215	1	0	10.295709	-0.067029	-4.215384
216	1	0	10.295706	3.868838	1.677719

$A_{Te}+A_{Te}$

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	8.310123	3.639366	-0.055580
2	6	0	7.714038	2.975838	-1.297111
3	6	0	7.719365	3.024064	1.211843
4	1	0	7.988864	4.684129	-0.075138
5	6	0	8.253606	1.813669	-1.872796
6	6	0	6.583160	3.531228	-1.917315
7	6	0	8.253586	1.871961	1.814329
8	6	0	6.599570	3.607821	1.824819
9	6	0	7.718917	1.211238	-3.024721

10	6	0	6.036752	2.983803	-3.076316
11	8	0	6.042516	4.733485	-1.401026
12	6	0	7.713681	1.296352	2.976388
13	6	0	6.036904	3.076018	2.984097
14	8	0	6.077274	4.818074	1.303814
15	6	0	8.309206	-0.056300	-3.640229
16	6	0	6.599058	1.824383	-3.608169
17	1	0	5.214191	3.474407	-3.581652
18	6	0	4.797688	4.708280	-0.764573
19	6	0	8.309535	0.054748	3.639998
20	6	0	6.582864	1.916827	3.531584
21	1	0	5.214397	3.581564	3.474580
22	6	0	4.816352	4.783748	0.694269
23	1	0	7.987634	-0.075716	-4.684898
24	6	0	7.713057	-1.297770	-2.976641
25	8	0	6.076329	1.303278	-4.818163
26	6	0	7.718848	-1.212624	3.024515
27	1	0	7.988013	0.074282	4.684683
28	8	0	6.041785	1.400734	4.733762
29	6	0	8.252760	-1.873516	-1.814581
30	6	0	6.582121	-1.917981	-3.531900
31	6	0	4.815325	0.693984	-4.783427
32	6	0	2.374261	4.754065	-0.749177
33	6	0	8.253276	-1.815225	1.872547
34	6	0	6.598818	-1.825393	3.608018
35	6	0	4.796953	0.764268	4.708092
36	6	0	2.388623	4.857500	0.734034
37	6	0	7.718246	-3.025538	-1.212155
38	6	0	6.035871	-3.077063	-2.984491
39	8	0	6.041139	-1.401588	-4.734001
40	6	0	4.796445	-0.764886	-4.708215
41	6	0	7.713217	-2.977130	1.296817
42	6	0	6.036036	-2.984583	3.076132
43	8	0	6.076412	-1.304138	4.818083
44	6	0	4.815523	-0.694577	4.783589
45	6	0	8.308921	-3.640931	0.055252
46	6	0	6.598359	-3.609039	-1.825191
47	1	0	5.213247	-3.582370	-3.475021
48	6	0	2.387549	0.734176	-4.856022
49	6	0	6.582130	-3.532104	1.917032
50	1	0	5.213339	-3.474917	3.581498
51	6	0	2.373502	0.749004	4.753243
52	1	0	7.987306	-4.685585	0.074904
53	8	0	6.075682	-4.819155	-1.304244
54	6	0	2.372989	-0.749100	-4.752977
55	8	0	6.041033	-4.734038	1.400524
56	6	0	2.387760	-0.734215	4.856868
57	6	0	4.814776	-4.784335	-0.694643
58	6	0	4.796182	-4.708434	0.764181
59	6	0	2.386986	-4.857200	-0.734334
60	6	0	2.372748	-4.753282	0.748857
61	6	0	3.626155	-1.465441	-4.704071
62	6	0	3.663937	1.416301	-4.879132
63	6	0	3.627500	4.704535	-1.465324
64	6	0	3.664884	4.880200	1.416374
65	6	0	3.663247	-4.880540	-1.416689
66	6	0	3.626018	-4.703973	1.464958
67	6	0	3.626805	1.465076	4.703980
68	6	0	3.663995	-1.416608	4.879818
69	1	0	3.621004	-2.549115	-4.713986
70	1	0	3.680291	2.492739	-5.004912
71	1	0	3.679431	-5.006824	-2.493071
72	1	0	3.622485	4.714267	-2.548996
73	1	0	3.621005	-4.713391	2.548635
74	1	0	3.681139	5.006227	2.492783
75	1	0	3.621886	2.548754	4.713700
76	1	0	3.680137	-2.493014	5.005896
77	7	0	1.177889	-4.681588	1.308015
78	7	0	1.211773	-4.872995	-1.337992
79	7	0	1.212560	-1.337855	4.872792
80	7	0	1.178635	1.308151	4.681789
81	7	0	1.213453	4.873612	1.337794
82	7	0	1.179362	4.683021	-1.308382
83	7	0	1.212487	1.338068	-4.871271
84	7	0	1.178019	-1.307990	-4.681522
85	1	0	9.128483	-1.413062	-1.366280
86	1	0	9.129315	1.365337	-1.412355
87	1	0	9.129255	1.411290	1.366148
88	1	0	9.129172	-1.367222	1.412122
89	6	0	9.847605	-3.612876	0.058704
90	1	0	10.228535	-4.105871	0.958475
91	1	0	10.257796	-2.597749	0.039167
92	6	0	9.848220	0.058278	3.611824
93	1	0	10.258345	0.038843	2.596673
94	1	0	10.233314	-0.819077	4.140649
95	6	0	9.848801	3.610784	-0.059175
96	1	0	10.258640	2.595519	-0.039684
97	1	0	10.234083	4.139559	0.818128
98	6	0	9.847889	-0.060282	-3.612096
99	1	0	10.258027	-0.041016	-2.596946
100	1	0	10.233241	0.816971	-4.140902
101	52	0	-0.359958	-0.023334	4.824539
102	52	0	-0.360684	-4.824328	-0.023429
103	52	0	-0.358951	4.825561	0.023313
104	52	0	-0.360360	0.023922	-4.823791
105	1	0	10.228535	-0.960120	-4.105178
106	1	0	10.232619	-4.141810	-0.818616
107	1	0	10.229133	0.958019	4.104873
108	1	0	10.229821	4.103671	-0.958962
109	6	0	-8.309066	-2.463000	-2.680837
110	6	0	-7.713423	-1.105155	-3.053026
111	6	0	-7.718621	-2.959776	-1.362344
112	1	0	-7.987052	-3.167338	-3.452419
113	6	0	-8.253142	0.112028	-2.605244
114	6	0	-6.582882	-1.036675	-3.883081
115	6	0	-8.253227	-2.605108	-0.111718
116	6	0	-6.598990	-3.806567	-1.364481
117	6	0	-7.718291	1.362578	-2.959833
118	6	0	-6.036478	0.181181	-4.282808
119	8	0	-6.042222	-2.238285	-4.400947
120	6	0	-7.713486	-3.052980	1.105425
121	6	0	-6.036848	-4.282926	-0.181115

122	8	0	-6.076695	-4.260460	-2.601494
123	6	0	-8.308481	2.681225	-2.463148
124	6	0	-6.598534	1.364591	-3.806449
125	1	0	-5.214398	0.210470	-4.987079
126	6	0	-4.797498	-2.682854	-3.944411
127	6	0	-8.309115	-2.680734	2.463261
128	6	0	-6.583061	-3.883184	1.036830
129	1	0	-5.214803	-4.987247	-0.210507
130	6	0	-4.815953	-3.794039	-2.996113
131	1	0	-7.986300	3.452688	-3.167537
132	6	0	-7.712776	3.053391	-1.105340
133	8	0	-6.076085	2.601623	-4.260003
134	6	0	-7.718642	-1.362210	2.959944
135	1	0	-7.987065	-3.452287	3.167621
136	8	0	-6.042273	-4.401352	2.238286
137	6	0	-8.252510	2.605546	0.111789
138	6	0	-6.582265	3.883514	-1.036767
139	6	0	-4.815359	2.996225	-3.793620
140	6	0	-2.373996	-2.724405	-3.966297
141	6	0	-8.253249	-0.111539	2.605369
142	6	0	-6.598845	-1.364435	3.806494
143	6	0	-4.797557	-3.944702	2.682829
144	6	0	-2.388101	-3.872947	-3.022107
145	6	0	-7.717876	2.960216	1.362425
146	6	0	-6.035985	4.283175	0.181158
147	8	0	-6.041537	4.401728	-2.238243
148	6	0	-4.796860	3.945071	-2.682926
149	6	0	-7.713196	1.105522	3.053013
150	6	0	-6.036413	-0.181129	4.282688
151	8	0	-6.076681	-2.601529	4.260202
152	6	0	-4.815975	-2.996213	3.793846
153	6	0	-8.308490	2.463518	2.680867
154	6	0	-6.598182	3.806888	1.364551
155	1	0	-5.213856	4.987405	0.210525
156	6	0	-2.387547	3.022078	-3.872502
157	6	0	-6.582539	1.036830	3.882934
158	1	0	-5.214233	-0.210599	4.986840
159	6	0	-2.374032	-3.966593	2.724277
160	1	0	-7.986355	3.167766	3.452483
161	8	0	-6.075803	4.260778	2.601536
162	6	0	-2.373333	3.967165	-2.724757
163	8	0	-6.041622	2.238363	4.400681
164	6	0	-2.388149	-3.022173	3.872615
165	6	0	-4.815150	3.794103	2.996119
166	6	0	-4.796816	2.682776	3.944266
167	6	0	-2.387314	3.872749	3.022149
168	6	0	-2.373299	2.724224	3.966356
169	6	0	-3.626671	4.423909	-2.171238
170	6	0	-3.663690	2.569377	-4.383694
171	6	0	-3.627342	-2.170749	-4.422823
172	6	0	-3.664291	-4.384408	-2.569690
173	6	0	-3.663422	4.384369	2.569747
174	6	0	-3.626716	2.170546	4.422695
175	6	0	-3.627417	-4.423218	2.170770
176	6	0	-3.664286	-2.569666	4.384063
177	1	0	-3.621761	5.176164	-1.391130
178	1	0	-3.679855	1.920492	-5.251734
179	1	0	-3.679514	5.252798	1.921370
180	1	0	-3.622408	-1.390274	-5.174698
181	1	0	-3.621851	1.390011	5.174507
182	1	0	-3.680435	-5.252801	-1.921267
183	1	0	-3.622560	-5.175199	1.390393
184	1	0	-3.680360	-1.921080	5.252334
185	7	0	-1.178547	2.268774	4.298931
186	7	0	-1.211986	4.321927	2.618907
187	7	0	-1.212880	-2.618703	4.321731
188	7	0	-1.179257	-4.299005	2.268776
189	7	0	-1.212828	-4.322340	-2.618947
190	7	0	-1.179232	-2.268952	-4.298780
191	7	0	-1.212297	2.618423	-4.321599
192	7	0	-1.178495	4.299997	-2.269622
193	1	0	-9.128282	1.963553	0.085769
194	1	0	-9.128951	0.086053	-1.963304
195	1	0	-9.128972	-1.963080	-0.085629
196	1	0	-9.129182	-0.085413	1.963588
197	6	0	-9.847190	2.442302	2.663252
198	1	0	-10.228005	2.128430	3.640085
199	1	0	-10.257769	1.758320	1.913097
200	6	0	-9.847813	-2.663214	2.441762
201	1	0	-10.258319	-1.913065	1.757738
202	1	0	-10.232714	-2.443751	3.442456
203	6	0	-9.847765	-2.441447	-2.663286
204	1	0	-10.258217	-1.757464	-1.913069
205	1	0	-10.232709	-3.442139	-2.443890
206	6	0	-9.847184	2.663986	-2.441594
207	1	0	-10.257778	1.913944	-1.757504
208	1	0	-10.232173	2.444541	-3.442257
209	52	0	0.360041	3.487148	-3.333858
210	52	0	0.359562	-3.333538	-3.486749
211	52	0	0.360299	3.333606	3.487280
212	52	0	0.359527	-3.486839	3.333398
213	1	0	-10.227710	3.640911	-2.127667
214	1	0	-10.228474	-2.127402	-3.640099
215	1	0	-10.228511	-3.640059	2.127806
216	1	0	-10.231892	3.443057	2.443749

RBr-RBr@A_{Se}+A_{Se}

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	8.359849	-1.372136	-3.367994
2	6	0	7.754229	-2.309450	-2.323631
3	6	0	7.780739	0.033987	-3.217241
4	1	0	8.035990	-1.741123	-4.344829
5	6	0	8.270059	-2.401246	-1.019985
6	6	0	6.657112	-3.129301	-2.632810
7	6	0	8.355510	1.028960	-2.407833
8	6	0	6.616618	0.375603	-3.922947
9	6	0	7.749973	-3.268084	-0.045639

10	6	0	6.102188	-3.998100	-1.693546
11	8	0	6.129529	-3.136400	-3.951860
12	6	0	7.806066	2.316900	-2.282324
13	6	0	6.055433	1.648782	-3.853300
14	8	0	6.070216	-0.580284	-4.808446
15	6	0	8.357066	-3.372445	1.351558
16	6	0	6.640852	-4.049979	-0.409324
17	1	0	5.289058	-4.658832	-1.970081
18	6	0	4.863461	-2.559168	-4.114601
19	6	0	8.405612	3.398555	-1.386750
20	6	0	6.642714	2.595782	-3.016938
21	1	0	5.212672	1.916078	-4.477196
22	6	0	4.832940	-1.157822	-4.522269
23	1	0	8.034214	-4.332194	1.763486
24	6	0	7.771914	-2.288121	2.251520
25	8	0	6.115004	-4.992672	0.508002
26	6	0	7.799506	3.299045	0.012253
27	1	0	8.089317	4.360404	-1.799094
28	8	0	6.127901	3.910778	-2.991453
29	6	0	8.325663	-1.002407	2.369279
30	6	0	6.618170	-2.564814	3.001102
31	6	0	4.856270	-4.754050	1.076383
32	6	0	2.452497	-2.608276	-4.057194
33	6	0	8.312509	2.428376	0.988250
34	6	0	6.691810	4.083044	0.372698
35	6	0	4.884344	4.175624	-2.410891
36	6	0	2.427897	-1.181810	-4.420686
37	6	0	7.772755	-0.010525	3.197202
38	6	0	6.050113	-1.620213	3.852652
39	8	0	6.094748	-3.876275	2.967607
40	6	0	4.845001	-4.125501	2.394100
41	6	0	7.779197	2.325751	2.283467
42	6	0	6.134186	4.018553	1.648524
43	8	0	6.180616	5.037399	-0.542403
44	6	0	4.914646	4.814134	-1.099256
45	6	0	8.367969	1.389299	3.337647
46	6	0	6.623102	-0.351829	3.926412
47	1	0	5.211286	-1.882809	4.484038
48	6	0	2.449540	-4.965330	1.147293
49	6	0	6.671720	3.135767	2.583731
50	1	0	5.320009	4.678662	1.922512
51	6	0	2.479078	4.355497	-2.446699
52	1	0	8.043971	1.770517	4.309736
53	8	0	6.094065	0.592705	4.835153
54	6	0	2.439848	-4.300393	2.459740
55	8	0	6.132905	3.123485	3.894347
56	6	0	2.508882	5.022506	-1.136362
57	6	0	4.849630	1.168677	4.561663
58	6	0	4.869820	2.543213	4.072972
59	6	0	2.440367	1.189960	4.538758
60	6	0	2.457216	2.582982	4.065697
61	6	0	3.680950	-3.902613	3.070200
62	6	0	3.706103	-5.174694	0.471224
63	6	0	3.720620	-3.279755	-3.923924
64	6	0	3.658245	-0.486552	-4.686237
65	6	0	3.680260	0.511484	4.805715
66	6	0	3.719771	3.244152	3.854616
67	6	0	3.711360	3.956036	-3.073692
68	6	0	3.774289	5.244568	-0.483837
69	1	0	3.670237	-3.494786	4.073035
70	1	0	3.725029	-5.700969	-0.475377
71	1	0	3.658234	-0.487310	5.222116
72	1	0	3.746812	-4.333828	-3.677538
73	1	0	3.734824	4.282286	3.547359
74	1	0	3.619426	0.536620	-5.036283
75	1	0	3.687919	3.544975	-4.075065
76	1	0	3.804996	5.773524	0.460668
77	7	0	1.262737	3.127321	3.848462
78	7	0	1.235755	0.648532	4.685985
79	7	0	1.319967	5.371600	-0.642072
80	7	0	1.267640	4.184107	-2.974463
81	7	0	1.223639	-0.626978	-4.477725
82	7	0	1.265252	-3.161763	-3.825701
83	7	0	1.256079	-5.340942	0.687793
84	7	0	1.241645	-4.146560	3.017890
85	1	0	9.223341	-0.768466	1.804385
86	1	0	9.121371	-1.779897	-0.756481
87	1	0	9.265062	0.796173	-1.861847
88	1	0	9.168317	1.810441	0.730990
89	6	0	9.906599	1.378802	3.314386
90	1	0	10.289278	2.392059	3.470751
91	1	0	10.318298	1.012869	2.367913
92	6	0	9.943293	3.365823	-1.364225
93	1	0	10.346380	2.433503	-0.955044
94	1	0	10.324695	4.187043	-0.749755
95	6	0	9.898271	-1.382448	-3.337101
96	1	0	10.309957	-1.034131	-2.384058
97	1	0	10.292892	-0.734123	-4.125725
98	6	0	9.895226	-3.353352	1.324429
99	1	0	10.305339	-2.422147	0.919711
100	1	0	10.268206	-4.174763	0.704945
101	1	0	10.335224	3.478962	-2.379893
102	1	0	10.267744	-2.398873	-3.503793
103	1	0	10.288329	0.734625	4.112638
104	1	0	10.288161	-3.475003	2.338661
105	34	0	-0.018169	4.891430	-1.838838
106	34	0	-0.076788	1.892888	4.249190
107	34	0	-0.082964	-1.896341	-4.087457
108	34	0	-0.061103	-4.869133	1.912731
109	6	0	-8.366655	-1.390183	3.336978
110	6	0	-7.777477	-2.326519	2.282806
111	6	0	-7.771647	0.009732	3.196702
112	1	0	-8.042758	-1.771418	4.309102
113	6	0	-8.310495	-2.429146	0.987467
114	6	0	-6.670068	-3.136562	2.583261
115	6	0	-8.324421	1.001514	2.368516
116	6	0	-6.621741	0.350914	3.925518
117	6	0	-7.797181	-3.299540	0.011369
118	6	0	-6.132336	-4.019221	1.648054
119	8	0	-6.131181	-3.124253	3.893822
120	6	0	-7.770072	2.286894	2.249887
121	6	0	-6.048236	1.619051	3.851034

122	8	0	-6.092614	-0.593535	4.834136
123	6	0	-8.402898	-3.398880	-1.387847
124	6	0	-6.689393	-4.083348	0.371951
125	1	0	-5.318167	-4.679318	1.922079
126	6	0	-4.868092	-2.543747	4.072054
127	6	0	-8.354968	3.371613	1.350275
128	6	0	-6.616045	2.563486	2.999136
129	1	0	-5.209183	1.881640	4.482104
130	6	0	-4.848037	-1.169127	4.560448
131	1	0	-8.086454	-4.360693	-1.800157
132	6	0	-7.803242	-2.317182	-2.283331
133	8	0	-6.177347	-5.037170	-0.543201
134	6	0	-7.747406	3.268144	-0.046762
135	1	0	-8.032347	4.331151	1.762888
136	8	0	-6.092942	3.875001	2.965743
137	6	0	-8.352431	-1.029119	-2.408709
138	6	0	-6.639931	-2.596213	-3.018031
139	6	0	-4.911407	-4.813130	-1.099906
140	6	0	-2.455516	-2.583087	4.064558
141	6	0	-8.267081	2.401301	-1.021337
142	6	0	-6.638853	4.050960	-0.410319
143	6	0	-4.843128	4.125243	2.392976
144	6	0	-2.438795	-1.189971	4.537228
145	6	0	-7.777308	-0.034071	-3.217857
146	6	0	-6.052450	-1.649229	-3.854206
147	8	0	-6.125072	-3.911156	-2.992399
148	6	0	-4.881320	-4.175443	-2.411954
149	6	0	-7.751144	2.309911	-2.324942
150	6	0	-6.100437	3.999824	-1.694695
151	8	0	-6.113035	4.993393	0.507250
152	6	0	-4.854300	4.754743	1.075673
153	6	0	-8.356240	1.372099	-3.369129
154	6	0	-6.613220	-0.375850	-3.923426
155	1	0	-5.209700	-1.916505	-4.478133
156	6	0	-2.505521	-5.020433	-1.136855
157	6	0	-6.654561	3.130537	-2.633960
158	1	0	-5.287656	4.661038	-1.971121
159	6	0	-2.438072	4.300977	2.459505
160	1	0	-8.032054	1.740708	-4.346003
161	8	0	-6.065994	0.580193	-4.808240
162	6	0	-2.475925	-4.354395	-2.447705
163	8	0	-6.125625	3.136728	-3.952391
164	6	0	-2.447588	4.966859	1.147499
165	6	0	-4.828948	1.157515	-4.520575
166	6	0	-4.859546	2.558896	-4.113073
167	6	0	-2.423885	1.181275	-4.418377
168	6	0	-2.448649	2.607338	-4.053819
169	6	0	-3.708421	-3.955762	-3.074896
170	6	0	-3.770855	-5.242564	-0.484167
171	6	0	-3.717959	-3.244504	3.853621
172	6	0	-3.678765	-0.511592	4.804057
173	6	0	-3.654235	0.486116	-4.684083
174	6	0	-3.716670	3.279101	-3.921249
175	6	0	-3.679233	3.902406	3.069338
176	6	0	-3.704073	5.176185	0.471156
177	1	0	-3.685141	-3.545350	-4.076544
178	1	0	-3.801326	-5.771001	0.460638
179	1	0	-3.615458	-0.536955	-5.034451
180	1	0	-3.732838	-4.282722	3.546644
181	1	0	-3.742707	4.333243	-3.675109
182	1	0	-3.656800	0.487165	5.220546
183	1	0	-3.668698	3.493855	4.071882
184	1	0	-3.722908	5.703096	-0.475104
185	7	0	-1.261635	3.160703	-3.821485
186	7	0	-1.219567	0.626642	-4.476031
187	7	0	-1.254074	5.342817	0.688424
188	7	0	-1.240003	4.146740	3.017759
189	7	0	-1.234196	-0.648610	4.684966
190	7	0	-1.260971	-3.127546	3.847995
191	7	0	-1.316567	-5.368972	-0.642372
192	7	0	-1.264540	-4.183146	-2.975630
193	1	0	-9.261898	-0.796190	-1.862604
194	1	0	-9.166228	-1.811165	0.730037
195	1	0	-9.222340	0.767593	1.804002
196	1	0	-9.118078	1.779436	-0.757989
197	6	0	-9.894688	1.382479	-3.338791
198	1	0	-10.289060	0.734241	-4.127607
199	6	0	-9.893126	3.352478	1.322565
200	1	0	-10.303047	2.421479	0.917188
201	1	0	-10.265914	4.174213	0.703398
202	6	0	-9.905272	-1.380000	3.313365
203	1	0	-10.316842	-1.014104	2.366820
204	1	0	-10.287333	-0.735968	4.111579
205	6	0	-9.940593	-3.366191	-1.365701
206	1	0	-10.343782	-2.433834	-0.956700
207	1	0	-10.322145	-4.187361	-0.751260
208	34	0	0.021442	-4.889445	-1.839524
209	34	0	0.078429	-1.893164	4.249017
210	34	0	0.086883	1.895960	-4.084836
211	34	0	0.062914	4.869817	1.913169
212	1	0	-10.286443	3.473572	2.336714
213	1	0	-10.306734	1.034058	-2.385939
214	1	0	-10.287767	-2.393351	3.469559
215	1	0	-10.332276	-3.479409	-2.381455
216	1	0	-10.264051	2.398940	-3.505525
217	6	0	-5.519445	-0.171768	0.136406
218	6	0	-4.374321	0.281405	-0.785890
219	1	0	-6.429568	-0.388753	-0.437150
220	1	0	-5.246742	-1.079966	0.692918
221	1	0	-5.763386	0.612499	0.867359
222	6	0	-3.122115	0.682149	0.022132
223	1	0	-4.123981	-0.522859	-1.494178
224	1	0	-4.710423	1.140880	-1.388527
225	1	0	-3.377955	1.510745	0.698093
226	1	0	-2.793171	-0.158092	0.647084
227	6	0	-1.987500	1.104966	-0.904212
228	1	0	-2.268970	1.945952	-1.542870
229	1	0	-1.593949	0.274454	-1.497559
230	35	0	-0.408316	1.792544	0.158849
231	6	0	1.953780	-1.083216	-0.904790
232	1	0	2.221510	-1.907859	-1.570072
233	1	0	1.557295	-0.234345	-1.469316

234	6	0	3.103118	-0.693109	0.017924
235	6	0	4.346171	-0.273129	-0.794438
236	1	0	3.364189	-1.542567	0.665413
237	1	0	2.786530	0.129467	0.672070
238	6	0	5.508068	0.140398	0.125776
239	1	0	4.667367	-1.113739	-1.430845
240	1	0	4.090847	0.556503	-1.470896
241	1	0	6.407775	0.383743	-0.453873
242	1	0	5.244927	1.022484	0.727055
243	1	0	5.765905	-0.675726	0.816020
244	35	0	0.384498	-1.790038	0.160209

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Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.338801	1.727262	-3.219434
2	6	0	-7.734189	2.553968	-2.085455
3	6	0	-7.760699	0.313350	-3.207788
4	1	0	-8.013346	2.192286	-4.153747
5	6	0	-8.246128	2.499205	-0.778677
6	6	0	-6.646768	3.414321	-2.307191
7	6	0	-8.340860	-0.760740	-2.511068
8	6	0	-6.588879	0.050420	-3.933781
9	6	0	-7.740558	3.268777	0.281456
10	6	0	-6.103559	4.187283	-1.281260
11	8	0	-6.114503	3.563270	-3.616195
12	6	0	-7.786892	-2.053152	-2.512474
13	6	0	-6.024769	-1.221702	-3.992290
14	8	0	-6.042186	1.096890	-4.708856
15	6	0	-8.360774	3.217216	1.676528
16	6	0	-6.644242	4.102136	0.001108
17	1	0	-5.296982	4.881757	-1.486293
18	6	0	-4.845525	3.009537	-3.834858
19	6	0	-8.389853	-3.226283	-1.741772
20	6	0	-6.616041	-2.250381	-3.261418
21	1	0	-5.176629	-1.421989	-4.633573
22	6	0	-4.808318	1.650371	-4.367286
23	1	0	-8.042715	4.125605	2.194965
24	6	0	-7.783568	2.039564	2.456474
25	8	0	-6.127855	4.957416	1.006712
26	6	0	-7.793150	-3.282541	-0.335872
27	1	0	-8.070519	-4.137284	-2.255104
28	8	0	-6.097582	-3.559546	-3.363258
29	6	0	-8.348242	0.752850	2.454021
30	6	0	-6.616851	2.231600	3.212621
31	6	0	-4.865353	4.664961	1.542804
32	6	0	-2.432853	3.071648	-3.787059
33	6	0	-8.312295	-2.522395	0.725762
34	6	0	-6.688106	-4.102248	-0.054007
35	6	0	-4.857580	-3.880093	-2.805268
36	6	0	-2.402488	1.683932	-4.276983
37	6	0	-7.788778	-0.322009	3.167041
38	6	0	-6.045770	1.203819	3.958941
39	8	0	-6.091290	3.537980	3.300001
40	6	0	-4.844257	3.854626	2.757418
41	6	0	-7.787966	-2.557836	2.028452
42	6	0	-6.140774	-4.175569	1.225734
43	8	0	-6.166679	-4.954427	-1.060335
44	6	0	-4.896356	-4.669175	-1.578661
45	6	0	-8.382146	-1.730317	3.168325
46	6	0	-6.627207	-0.062180	3.910743
47	1	0	-5.199240	1.397003	4.604437
48	6	0	-2.459700	4.887370	1.635965
49	6	0	-6.683914	-3.398402	2.247514
50	1	0	-5.327444	-4.860909	1.432701
51	6	0	-2.452154	-4.047617	-2.840624
52	1	0	-8.059761	-2.204811	4.099104
53	8	0	-6.097299	-1.097283	4.712447
54	6	0	-2.440043	4.026038	2.829282
55	8	0	-6.147945	-3.530758	3.553333
56	6	0	-2.489590	-4.872275	-1.623356
57	6	0	-4.854882	-1.648639	4.387737
58	6	0	-4.881221	-2.978767	3.789853
59	6	0	-2.446363	-1.687849	4.376484
60	6	0	-2.468135	-3.041546	3.801374
61	6	0	-3.674891	3.537699	3.384054
62	6	0	-3.722313	5.182275	1.002817
63	6	0	-3.705838	3.718867	-3.587820
64	6	0	-3.629429	1.005500	-4.595809
65	6	0	-3.681991	-1.020728	4.686034
66	6	0	-3.734886	-3.671022	3.525620
67	6	0	-3.679938	-3.576886	-3.424862
68	6	0	-3.759929	-5.169961	-1.010536
69	1	0	-3.652559	2.988726	4.316880
70	1	0	-3.751355	5.836670	0.140070
71	1	0	-3.652558	-0.059236	5.181957
72	1	0	-3.738867	4.745865	-3.246042
73	1	0	-3.757546	-4.681205	3.136317
74	1	0	-3.584703	0.018213	-5.036689
75	1	0	-3.647786	-3.049275	-4.369724
76	1	0	-3.797531	-5.807684	-0.136015
77	7	0	-1.273553	-3.580869	3.562480
78	7	0	-1.239486	-1.168614	4.579837
79	7	0	-1.303416	-5.285850	-1.172978
80	7	0	-1.238896	-3.813935	-3.338685
81	7	0	-1.196594	1.141004	-4.385792
82	7	0	-1.247276	3.607863	-3.508265
83	7	0	-1.270947	5.335112	1.232645
84	7	0	-1.239537	3.787808	3.348579
85	1	0	-9.255907	0.582931	1.882155
86	1	0	-9.085491	1.838172	-0.581293
87	1	0	-9.257330	-0.587438	-1.954376
88	1	0	-9.163580	-1.876200	0.529656
89	6	0	-9.920515	-1.720972	3.140871
90	1	0	-10.301141	-2.745433	3.196288
91	1	0	-10.329782	-1.265751	2.232873
92	6	0	-9.927682	-3.196580	-1.724997
93	1	0	-10.334089	-2.314658	-1.218879

94	1	0	-10.311979	-4.080095	-1.206232
95	6	0	-9.877219	1.737095	-3.189274
96	1	0	-10.290575	1.297660	-2.275423
97	1	0	-10.272060	1.170279	-4.038310
98	6	0	-9.898517	3.203158	1.631252
99	1	0	-10.304555	2.324260	1.119631
100	1	0	-10.264648	4.089631	1.104375
101	34	0	0.040235	-4.662554	-2.297159
102	34	0	0.067305	-2.390075	4.075852
103	34	0	0.104495	2.375156	-3.884019
104	34	0	0.055707	4.673676	2.358561
105	1	0	-10.313638	-3.198177	-2.749226
106	1	0	-10.244648	2.765671	-3.255396
107	1	0	-10.306842	-1.158370	3.996540
108	1	0	-10.302315	3.210504	2.648537
109	6	0	8.356176	1.056727	3.468550
110	6	0	7.774192	2.094803	2.509611
111	6	0	7.765934	-0.323989	3.187920
112	1	0	8.025077	1.339389	4.471491
113	6	0	8.318564	2.334431	1.237289
114	6	0	6.662873	2.867972	2.883393
115	6	0	8.323096	-1.224321	2.263812
116	6	0	6.618299	-0.743801	3.878279
117	6	0	7.813585	3.303845	0.354461
118	6	0	6.134340	3.846883	2.043604
119	8	0	6.109228	2.711169	4.178023
120	6	0	7.776665	-2.494839	2.016760
121	6	0	6.051281	-2.000867	3.675091
122	8	0	6.078832	0.101489	4.875070
123	6	0	8.429231	3.544939	-1.023134
124	6	0	6.703577	4.047279	0.786891
125	1	0	5.318054	4.475209	2.379077
126	6	0	4.849148	2.106257	4.276764
127	6	0	8.369238	-3.477048	1.011266
128	6	0	6.624104	-2.852339	2.733585
129	1	0	5.211931	-2.329906	4.273976
130	6	0	4.833492	0.693846	4.641230
131	1	0	8.117952	4.544934	-1.336716
132	6	0	7.831213	2.561438	-2.026696
133	8	0	6.201786	5.096978	-0.022985
134	6	0	7.764055	-3.227706	-0.367790
135	1	0	8.049627	-4.475975	1.319410
136	8	0	6.108330	-4.157958	2.573503
137	6	0	8.380086	1.292951	-2.284690
138	6	0	6.666744	2.914332	-2.727296
139	6	0	4.937408	4.944754	-0.607135
140	6	0	2.437706	2.124042	4.221857
141	6	0	8.285514	-2.265830	-1.247419
142	6	0	6.652943	-3.965994	-0.808640
143	6	0	4.858667	-4.361685	1.981956
144	6	0	2.424991	0.695678	4.573869
145	6	0	7.801549	0.384824	-3.188765
146	6	0	6.078296	2.058509	-3.655599
147	8	0	6.155598	4.220972	-2.569392
148	6	0	4.909801	4.436743	-1.974135
149	6	0	7.768500	-2.038264	-2.533989
150	6	0	6.114606	-3.781809	-2.080336
151	8	0	6.129722	-4.998278	0.007679
152	6	0	4.870857	-4.835806	0.600571
153	6	0	8.376313	-1.001285	-3.478706
154	6	0	6.637655	0.798303	-3.855245
155	1	0	5.234973	2.388931	-4.247661
156	6	0	2.535643	5.196022	-0.644043
157	6	0	6.670068	-2.820363	-2.924514
158	1	0	5.301812	-4.410265	-2.424439
159	6	0	2.456958	-4.593693	2.045102
160	1	0	8.051778	-1.270021	-4.487589
161	8	0	6.087730	-0.060398	-4.833544
162	6	0	2.507659	4.656391	-2.011130
163	8	0	6.138874	-2.687844	-4.234910
164	6	0	2.468505	-5.097175	0.661862
165	6	0	4.848425	-0.658661	-4.602222
166	6	0	4.874466	-2.092054	-4.329361
167	6	0	2.443977	-0.681758	-4.488993
168	6	0	2.464635	-2.134776	-4.253530
169	6	0	3.739204	4.297757	-2.663372
170	6	0	3.797515	5.332088	0.037825
171	6	0	3.696358	2.812776	4.095760
172	6	0	3.666792	0.007815	4.805131
173	6	0	3.676017	0.029755	-4.697108
174	6	0	3.729623	-2.821670	-4.194822
175	6	0	3.696610	-4.241352	2.687392
176	6	0	3.722828	-5.202394	-0.042245
177	1	0	3.718780	3.985354	-3.699883
178	1	0	3.827506	5.768417	1.028590
179	1	0	3.640170	1.081300	-4.949978
180	1	0	3.704829	3.873703	3.879812
181	1	0	3.751118	-3.894248	-4.048427
182	1	0	3.647740	-1.024406	5.129927
183	1	0	3.688828	-3.951488	3.730638
184	1	0	3.741759	-5.616593	-1.042911
185	7	0	1.276760	-2.702715	-4.064189
186	7	0	1.242035	-0.118978	-4.489031
187	7	0	1.279544	-5.441781	0.166931
188	7	0	1.260866	-4.535351	2.627338
189	7	0	1.223173	0.134481	4.651988
190	7	0	1.243370	2.676272	4.029665
191	7	0	1.346786	5.521503	-0.129573
192	7	0	1.297881	4.558378	-2.564883
193	1	0	9.291651	1.005534	-1.768450
194	1	0	9.176155	1.746197	0.922650
195	1	0	9.218242	-0.929021	1.724067
196	1	0	9.138051	-1.676252	-0.921983
197	6	0	9.914647	-1.019262	-3.448600
198	1	0	10.311697	-0.296762	-4.168528
199	6	0	9.907341	-3.449781	0.991331
200	1	0	10.315473	-2.479982	0.688179
201	1	0	10.285126	-4.200403	0.290303
202	6	0	9.895075	1.050162	3.454923
203	1	0	10.313401	0.779095	2.479885
204	1	0	10.272547	0.331132	4.188644
205	6	0	9.966570	3.505520	-0.995445

206	1	0	10.365357	2.535694	-0.680050
207	1	0	10.346223	4.259564	-0.299245
208	34	0	0.016656	5.180845	-1.378651
209	34	0	-0.093020	1.403431	4.299826
210	34	0	-0.067437	-1.414180	-4.206852
211	34	0	-0.035230	-5.146652	1.448092
212	1	0	10.297634	-3.675912	1.988506
213	1	0	10.326555	-0.768766	-2.465414
214	1	0	10.275044	2.043623	3.712277
215	1	0	10.364661	3.719352	-1.992341
216	1	0	10.281267	-2.015155	-3.715411
217	6	0	5.601892	0.216210	0.133948
218	6	0	4.435960	-0.117504	-0.812691
219	1	0	6.530398	0.396245	-0.421956
220	1	0	5.386180	1.113354	0.731729
221	1	0	5.787874	-0.616028	0.828692
222	6	0	3.180583	-0.542703	-0.023102
223	1	0	4.208023	0.750498	-1.449469
224	1	0	4.733316	-0.936645	-1.487455
225	1	0	3.417123	-1.445964	0.557545
226	1	0	2.907905	0.240112	0.697154
227	6	0	2.001705	-0.817746	-0.956840
228	1	0	2.250394	-1.564698	-1.715613
229	1	0	1.609664	0.090426	-1.424376
230	53	0	0.316314	-1.688121	0.132611
231	6	0	-2.237071	1.280261	-0.850658
232	1	0	-2.579578	2.148383	-1.418347
233	1	0	-1.829854	0.512241	-1.514712
234	6	0	-3.322864	0.747090	0.074590
235	6	0	-4.579199	0.355865	-0.729456
236	1	0	-3.591619	1.515890	0.813868
237	1	0	-2.945244	-0.120627	0.631220
238	6	0	-5.674176	-0.208047	0.189162
239	1	0	-4.965777	1.243646	-1.256184
240	1	0	-4.318147	-0.382279	-1.502735
241	1	0	-6.604680	-0.387478	-0.362866
242	1	0	-5.361683	-1.158855	0.644731
243	1	0	-5.896432	0.499985	0.999488
244	35	0	-0.656711	1.960432	0.208986

RI-RI@A_{Se}+A_{Se}

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.336837	1.553570	-3.288643
2	6	0	-7.733930	2.431618	-2.192735
3	6	0	-7.761748	0.140278	-3.212507
4	1	0	-8.008487	1.974735	-4.242566
5	6	0	-8.250614	2.443189	-0.886757
6	6	0	-6.643236	3.277284	-2.452458
7	6	0	-8.344974	-0.899544	-2.468064
8	6	0	-6.590933	-0.159129	-3.926228
9	6	0	-7.746838	3.264008	0.135303
10	6	0	-6.101448	4.099134	-1.464584
11	8	0	-6.109309	3.361837	-3.766020
12	6	0	-7.794926	-2.192374	-2.409866
13	6	0	-6.031848	-1.434740	-3.927849
14	8	0	-6.039133	0.849170	-4.746906
15	6	0	-8.368548	3.279149	1.530465
16	6	0	-6.648199	4.080544	-0.182122
17	1	0	-5.291687	4.779867	-1.700727
18	6	0	-4.840817	2.797302	-3.957142
19	6	0	-8.401461	-3.325972	-1.584108
20	6	0	-6.625325	-2.427176	-3.149974
21	1	0	-5.184028	-1.666112	-4.559193
22	6	0	-4.804762	1.415725	-4.428057
23	1	0	-8.051346	4.211105	2.005809
24	6	0	-7.788683	2.139533	2.363175
25	8	0	-6.138216	4.988944	0.779603
26	6	0	-7.804958	-3.316438	-0.176907
27	1	0	-8.084138	-4.261198	-2.053276
28	8	0	-6.109991	-3.740866	-3.193075
29	6	0	-8.352950	0.853981	2.422008
30	6	0	-6.618425	2.366745	3.104367
31	6	0	-4.875012	4.737500	1.333404
32	6	0	-2.428442	2.861048	-3.912175
33	6	0	-8.323294	-2.508307	0.849252
34	6	0	-6.697186	-4.119537	0.140243
35	6	0	-4.870353	-4.040991	-2.622623
36	6	0	-2.398698	1.453107	-4.340964
37	6	0	-7.790661	-0.187327	3.181390
38	6	0	-6.044726	1.374614	3.895191
39	8	0	-6.096605	3.677289	3.133189
40	6	0	-4.850032	3.983607	2.584751
41	6	0	-7.793440	-2.477949	2.150089
42	6	0	-6.145302	-4.129493	1.420081
43	8	0	-6.180612	-5.020998	-0.824429
44	6	0	-4.910223	-4.770362	-1.360049
45	6	0	-8.383356	-1.594891	3.250536
46	6	0	-6.627237	0.108022	3.908685
47	1	0	-5.195554	1.597281	4.527634
48	6	0	-2.473522	5.002325	1.430846
49	6	0	-6.686164	-3.304295	2.404883
50	1	0	-5.329959	-4.802590	1.657165
51	6	0	-2.466494	-4.233280	-2.661219
52	1	0	-8.057937	-2.024058	4.202076
53	8	0	-6.094338	-0.887933	4.756669
54	6	0	-2.448730	4.200246	2.666137
55	8	0	-6.143250	-3.371482	3.712871
56	6	0	-2.505880	-5.002786	-1.408966
57	6	0	-4.851690	-1.449513	4.451841
58	6	0	-4.876739	-2.805487	3.915223
59	6	0	-2.443533	-1.476874	4.421723
60	6	0	-2.463510	-2.855452	3.908822
61	6	0	-3.680539	3.716479	3.233949
62	6	0	-3.736844	5.247128	0.777069
63	6	0	-3.701062	3.516122	-3.740519
64	6	0	-3.626012	0.760675	-4.627050
65	6	0	-3.679978	-0.803240	4.712512

66	6	0	-3.729139	-3.503657	3.673673
67	6	0	-3.692471	-3.777011	-3.260181
68	6	0	-3.775389	-5.256094	-0.775163
69	1	0	-3.656460	3.212384	4.191751
70	1	0	-3.769681	5.859669	-0.115655
71	1	0	-3.651694	0.179855	5.163993
72	1	0	-3.733841	4.557032	-3.444053
73	1	0	-3.749165	-4.530472	3.330631
74	1	0	-3.581819	-0.245769	-5.022446
75	1	0	-3.660467	-3.294833	-4.229027
76	1	0	-3.814946	-5.852767	0.127806
77	7	0	-1.268898	-3.399665	3.683235
78	7	0	-1.238146	-0.942195	4.589980
79	7	0	-1.321540	-5.416127	-0.949998
80	7	0	-1.253333	-4.037737	-3.178899
81	7	0	-1.193079	0.905540	-4.428523
82	7	0	-1.242386	3.410900	-3.661847
83	7	0	-1.289927	5.447952	1.010483
84	7	0	-1.248943	4.006813	3.205434
85	1	0	-9.262568	0.658162	1.861656
86	1	0	-9.092232	1.794813	-0.659129
87	1	0	-9.260493	-0.698168	-1.919270
88	1	0	-9.176487	-1.873930	0.624822
89	6	0	-9.921840	-1.586646	3.227571
90	1	0	-10.302263	-2.607132	3.334221
91	1	0	-10.333967	-1.176394	2.299638
92	6	0	-9.939148	-3.291319	-1.569638
93	1	0	-10.343289	-2.385934	-1.104794
94	1	0	-10.326141	-4.148880	-1.010836
95	6	0	-9.875357	1.567155	-3.262626
96	1	0	-10.291564	1.170769	-2.330545
97	1	0	-10.269192	0.962624	-4.085727
98	6	0	-9.906082	3.260991	1.485602
99	1	0	-10.310806	2.359760	1.013311
100	1	0	-10.273192	4.122543	0.919525
101	1	0	-10.324708	-3.338969	-2.592903
102	1	0	-10.240884	2.592224	-3.376694
103	1	0	-10.305518	-0.982801	4.055897
104	1	0	-10.310354	3.313095	2.501402
105	34	0	0.018624	-4.861453	-2.111066
106	34	0	0.070482	-2.179346	4.128552
107	34	0	0.107802	2.162981	-3.986829
108	34	0	0.039359	4.861195	2.175451
109	6	0	8.360953	1.217403	3.419409
110	6	0	7.779433	2.210964	2.413165
111	6	0	7.771050	-0.175434	3.201582
112	1	0	8.028725	1.545525	4.408068
113	6	0	8.322871	2.386899	1.129904
114	6	0	6.669128	3.003695	2.747993
115	6	0	8.333871	-1.124127	2.330362
116	6	0	6.613568	-0.555161	3.898681
117	6	0	7.817229	3.309572	0.198313
118	6	0	6.140652	3.938663	1.859503
119	8	0	6.113327	2.916989	4.048821
120	6	0	7.779591	-2.400670	2.137749
121	6	0	6.039746	-1.817039	3.751244
122	8	0	6.073557	0.340631	4.848840
123	6	0	8.430142	3.477789	-1.191600
124	6	0	6.708020	4.074819	0.593655
125	1	0	5.324420	4.583154	2.163306
126	6	0	4.850403	2.322467	4.174769
127	6	0	8.368190	-3.435820	1.184327
128	6	0	6.616359	-2.715787	2.857374
129	1	0	5.193576	-2.112075	4.357937
130	6	0	4.830084	0.924072	4.588980
131	1	0	8.118818	4.460506	-1.555874
132	6	0	7.829811	2.444630	-2.143146
133	8	0	6.205657	5.084158	-0.265897
134	6	0	7.757341	-3.258875	-0.203898
135	1	0	8.048509	-4.416644	1.546035
136	8	0	6.100874	-4.026173	2.754744
137	6	0	8.378803	1.165262	-2.340141
138	6	0	6.662537	2.761109	-2.856389
139	6	0	4.939469	4.906209	-0.839142
140	6	0	2.438321	2.349947	4.129845
141	6	0	8.273492	-2.336702	-1.128414
142	6	0	6.651454	-4.024560	-0.610194
143	6	0	4.853107	-4.271477	2.176921
144	6	0	2.422174	0.933521	4.526600
145	6	0	7.797269	0.213026	-3.195361
146	6	0	6.071677	1.860316	-3.740088
147	8	0	6.151630	4.073533	-2.760743
148	6	0	4.907551	4.322378	-2.175258
149	6	0	7.759954	-2.176221	-2.426155
150	6	0	6.112452	-3.902137	-1.889526
151	8	0	6.134009	-5.025019	0.249257
152	6	0	4.872833	-4.841585	0.831971
153	6	0	8.369679	-1.186207	-3.418917
154	6	0	6.630799	0.591912	-3.877780
155	1	0	5.226306	2.160628	-4.345176
156	6	0	2.538941	5.173744	-0.889643
157	6	0	6.665240	-2.981333	-2.779630
158	1	0	5.301247	-4.548990	-2.202652
159	6	0	2.453508	-4.520589	2.250450
160	1	0	8.045027	-1.502007	-4.413999
161	8	0	6.080870	-0.316984	-4.809002
162	6	0	2.506712	4.553765	-2.222154
163	8	0	6.135421	-2.916975	-4.095873
164	6	0	2.473161	-5.128329	0.909233
165	6	0	4.842570	-0.906575	-4.553148
166	6	0	4.870314	-2.328013	-4.222373
167	6	0	2.437632	-0.932473	-4.451878
168	6	0	2.459443	-2.374915	-4.159755
169	6	0	3.734936	4.149436	-2.853256
170	6	0	3.802488	5.337244	-0.216448
171	6	0	3.699883	3.027877	3.973897
172	6	0	3.661197	0.248212	4.776935
173	6	0	3.668829	-0.226098	-4.681114
174	6	0	3.726390	-3.055249	-4.066885
175	6	0	3.687976	-4.111015	2.868764
176	6	0	3.730943	-5.268928	0.216372
177	1	0	3.710692	3.779338	-3.870467

178	1	0	3.837115	5.829533	0.747603
179	1	0	3.630963	0.814529	-4.975476
180	1	0	3.713156	4.080764	3.721677
181	1	0	3.750930	-4.120874	-3.876368
182	1	0	3.637483	-0.771396	5.138909
183	1	0	3.673103	-3.748300	3.888838
184	1	0	3.757804	-5.751969	-0.752799
185	7	0	1.272054	-2.937087	-3.949926
186	7	0	1.235762	-0.370517	-4.477100
187	7	0	1.289220	-5.520418	0.438161
188	7	0	1.256327	-4.426161	2.824409
189	7	0	1.218924	0.378840	4.630968
190	7	0	1.244064	2.902021	3.929774
191	7	0	1.352867	5.547072	-0.398992
192	7	0	1.297239	4.436117	-2.773934
193	1	0	9.291456	0.903679	-1.812542
194	1	0	9.178812	1.781702	0.844101
195	1	0	9.237489	-0.861828	1.787866
196	1	0	9.121118	-1.726255	-0.829668
197	6	0	9.908039	-1.205928	-3.387363
198	1	0	10.306830	-0.518027	-4.139533
199	6	0	9.906102	-3.411387	1.155885
200	1	0	10.313559	-2.459851	0.798622
201	1	0	10.279952	-4.199156	0.494671
202	6	0	9.899780	1.211329	3.407173
203	1	0	10.319036	0.897913	2.445292
204	1	0	10.277355	0.525757	4.172238
205	6	0	9.967463	3.438203	-1.164653
206	1	0	10.365636	2.485291	-0.800562
207	1	0	10.349196	4.226518	-0.508711
208	34	0	0.023322	5.146045	-1.630945
209	34	0	-0.093585	1.642018	4.252394
210	34	0	-0.072152	-1.655050	-4.144434
211	34	0	-0.031619	-5.133099	1.689335
212	1	0	10.300989	-3.583915	2.161972
213	1	0	10.320185	-0.911641	-2.416458
214	1	0	10.278891	2.215457	3.620594
215	1	0	10.364086	3.600136	-2.171873
216	1	0	10.272680	-2.213752	-3.608108
217	6	0	5.680429	0.242951	0.156634
218	6	0	4.551945	-0.171666	-0.800885
219	1	0	6.607008	0.463455	-0.386388
220	1	0	5.403927	1.138483	0.731748
221	1	0	5.895115	-0.565064	0.870280
222	6	0	3.296117	-0.603349	-0.017881
223	1	0	4.307301	0.658126	-1.480806
224	1	0	4.894339	-1.009210	-1.430392
225	1	0	3.557103	-1.449283	0.634564
226	1	0	2.963015	0.214864	0.634556
227	6	0	2.164878	-1.005686	-0.962108
228	1	0	2.471958	-1.804828	-1.641682
229	1	0	1.758107	-0.157502	-1.521532
230	53	0	0.479350	-1.847100	0.143357
231	6	0	-2.255965	1.018669	-0.941160
232	1	0	-2.589145	1.818542	-1.606711
233	1	0	-1.844721	0.185251	-1.518595
234	6	0	-3.368836	0.590269	0.012020
235	6	0	-4.638959	0.192516	-0.764693
236	1	0	-3.616012	1.416609	0.694380
237	1	0	-3.027519	-0.248644	0.633232
238	6	0	-5.749174	-0.259602	0.195166
239	1	0	-4.990645	1.057157	-1.351125
240	1	0	-4.409426	-0.606719	-1.485120
241	1	0	-6.692123	-0.432968	-0.336174
242	1	0	-5.474443	-1.191299	0.710565
243	1	0	-5.931274	0.509948	0.958124
244	53	0	-0.570030	1.876578	0.147395

RBr-RBr@$\mathbf{A_{Se}}$+$\mathbf{A_{Te}}$

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.333448	1.264074	-3.432410
2	6	0	-7.729264	2.233112	-2.416919
3	6	0	-7.760414	-0.138562	-3.235362
4	1	0	-8.004230	1.600503	-4.419196
5	6	0	-8.250228	2.371379	-1.119653
6	6	0	-6.627740	3.037911	-2.749610
7	6	0	-8.336797	-1.101435	-2.389262
8	6	0	-6.600680	-0.510322	-3.933250
9	6	0	-7.732699	3.271122	-0.173848
10	6	0	-6.075590	3.938100	-1.838966
11	8	0	-6.092104	2.993739	-4.063230
12	6	0	-7.794419	-2.387740	-2.220573
13	6	0	-6.046869	-1.783252	-3.820499
14	8	0	-6.047799	0.411615	-4.849714
15	6	0	-8.349902	3.426337	1.214414
16	6	0	-6.620419	4.038120	-0.560078
17	1	0	-5.258040	4.585087	-2.134211
18	6	0	-4.828124	2.401927	-4.199860
19	6	0	-8.400309	-3.432653	-1.285976
20	6	0	-6.635749	-2.698433	-2.950178
21	1	0	-5.204402	-2.075541	-4.433571
22	6	0	-4.806209	0.990334	-4.575620
23	1	0	-8.025158	4.398501	1.594741
24	6	0	-7.777882	2.372362	2.157878
25	8	0	-6.093849	5.011890	0.323373
26	6	0	-7.804360	-3.282799	0.113043
27	1	0	-8.082539	-4.409905	-1.659303
28	8	0	-6.120373	-4.011872	-2.881539
29	6	0	-8.338746	1.094614	2.322542
30	6	0	-6.625125	2.671630	2.900492
31	6	0	-4.837250	4.782865	0.904106
32	6	0	-2.403117	2.443432	-4.137914
33	6	0	-8.326260	-2.385232	1.059638
34	6	0	-6.692927	-4.047979	0.501767
35	6	0	-4.875128	-4.245010	-2.286292
36	6	0	-2.387398	0.994828	-4.481069
37	6	0	-7.792195	0.130794	3.187741

38	6	0	-6.065852	1.757270	3.789536
39	8	0	-6.092636	3.976457	2.816737
40	6	0	-4.836776	4.193137	2.240755
41	6	0	-7.796150	-2.236161	2.352095
42	6	0	-6.141412	-3.940831	1.776952
43	8	0	-6.172356	-5.024009	-0.382747
44	6	0	-4.904366	-4.813170	-0.942086
45	6	0	-8.388358	-1.264003	3.372174
46	6	0	-6.644168	0.494867	3.908745
47	1	0	-5.226606	2.038665	4.411858
48	6	0	-2.415842	4.979972	0.972243
49	6	0	-6.685976	-3.031268	2.681897
50	1	0	-5.324031	-4.586276	2.074601
51	6	0	-2.455952	-4.413601	-2.318071
52	1	0	-8.067364	-1.612599	4.357527
53	8	0	-6.117092	-0.416976	4.850351
54	6	0	-2.418166	4.340864	2.315206
55	8	0	-6.147388	-2.974220	3.990633
56	6	0	-2.485166	-5.006838	-0.955808
57	6	0	-4.868482	-0.996473	4.596169
58	6	0	-4.883734	-2.385582	4.148568
59	6	0	-2.446645	-1.003396	4.580238
60	6	0	-2.457758	-2.425202	4.144586
61	6	0	-3.677081	3.976239	2.922566
62	6	0	-3.680944	5.172762	0.293881
63	6	0	-3.680319	3.113826	-4.019950
64	6	0	-3.635789	0.311408	-4.723519
65	6	0	-3.701612	-0.330844	4.818849
66	6	0	-3.730666	-3.084659	3.950647
67	6	0	-3.702188	-4.055480	-2.955290
68	6	0	-3.761636	-5.194800	-0.302977
69	1	0	-3.673633	3.596274	3.936881
70	1	0	-3.691652	5.669698	-0.669208
71	1	0	-3.683916	0.680467	5.205529
72	1	0	-3.699270	4.173393	-3.794890
73	1	0	-3.741729	-4.131861	3.673368
74	1	0	-3.606069	-0.720057	-5.051423
75	1	0	-3.680594	-3.696819	-3.977278
76	1	0	-3.789536	-5.671869	0.669363
77	7	0	-1.280863	-2.997457	3.940168
78	7	0	-1.264191	-0.427454	4.721128
79	7	0	-1.316217	-5.322797	-0.411203
80	7	0	-1.263720	-4.255221	-2.878456
81	7	0	-1.206599	0.407269	-4.535588
82	7	0	-1.234749	3.018739	-3.906671
83	7	0	-1.237134	5.336265	0.479821
84	7	0	-1.243299	4.165248	2.899601
85	1	0	-9.234312	0.842941	1.761725
86	1	0	-9.103629	1.760797	-0.838018
87	1	0	-9.241944	-0.843678	-1.846841
88	1	0	-9.183814	-1.779575	0.779680
89	6	0	-9.926815	-1.253418	3.342935
90	1	0	-10.311040	-2.260960	3.529868
91	1	0	-10.334287	-0.917480	2.383565
92	6	0	-9.938148	-3.396866	-1.275764
93	1	0	-10.342179	-2.448506	-0.906194
94	1	0	-10.325478	-4.192913	-0.632411
95	6	0	-9.871997	1.280301	-3.407882
96	1	0	-10.288060	0.962956	-2.445925
97	1	0	-10.265699	0.608623	-4.177246
98	6	0	-9.887898	3.413656	1.175511
99	1	0	-10.299140	2.470032	0.801817
100	1	0	-10.251936	4.213508	0.523274
101	1	0	-10.323025	-3.548505	-2.289149
102	1	0	-10.237644	2.292275	-3.607364
103	1	0	-10.311096	-0.583483	4.118510
104	1	0	-10.288205	3.573946	2.181532
105	52	0	0.210937	-4.927808	-1.673120
106	52	0	0.246038	-1.715597	4.330688
107	52	0	0.303502	1.710273	-4.165732
108	52	0	0.262041	4.879681	1.763672
109	6	0	8.297137	1.490458	3.302669
110	6	0	7.714190	2.391449	2.214893
111	6	0	7.701641	0.087087	3.206963
112	1	0	7.969358	1.904551	4.259924
113	6	0	8.255443	2.451887	0.920362
114	6	0	6.605958	3.212005	2.481780
115	6	0	8.256348	-0.932068	2.414113
116	6	0	6.549920	-0.229413	3.943818
117	6	0	7.751308	3.292604	-0.086246
118	6	0	6.077592	4.067150	1.516431
119	8	0	6.058727	3.242834	3.789121
120	6	0	7.702937	-2.221269	2.338639
121	6	0	5.977845	-1.499792	3.913114
122	8	0	6.016996	0.746426	4.817216
123	6	0	8.368174	3.343766	-1.483469
124	6	0	6.644331	4.091376	0.242948
125	1	0	5.264698	4.739198	1.764628
126	6	0	4.796599	2.668962	3.984114
127	6	0	8.289034	-3.334861	1.475799
128	6	0	6.548779	-2.472568	3.095957
129	1	0	5.138478	-1.741368	4.552299
130	6	0	4.774822	1.312773	4.520353
131	1	0	8.056728	4.291557	-1.930643
132	6	0	7.772929	2.232781	-2.345838
133	8	0	6.140221	5.020386	-0.702516
134	6	0	7.686997	-3.273574	0.073773
135	1	0	7.963061	-4.280499	1.916883
136	8	0	6.024809	-3.784971	3.106782
137	6	0	8.322110	0.941156	-2.429195
138	6	0	6.611147	2.487956	-3.091117
139	6	0	4.877510	4.777762	-1.258078
140	6	0	2.383701	2.713213	3.983778
141	6	0	8.215291	-2.442674	-0.927082
142	6	0	6.575223	-4.061550	-0.268314
143	6	0	4.775831	-4.046964	2.539811
144	6	0	2.365453	1.338681	4.502596
145	6	0	7.745777	-0.079916	-3.204672
146	6	0	6.023814	1.515365	-3.897098
147	8	0	6.097286	3.803257	-3.106857
148	6	0	4.852284	4.085519	-2.540410
149	6	0	7.705761	-2.392379	-2.235635

150	6	0	6.043752	-4.052229	-1.556336
151	8	0	6.039652	-4.969616	0.678594
152	6	0	4.783423	-4.705803	1.238164
153	6	0	8.320733	-1.492240	-3.307153
154	6	0	6.582563	0.239669	-3.921873
155	1	0	5.184412	1.763612	-4.533203
156	6	0	2.472278	4.982094	-1.313169
157	6	0	6.607204	-3.218437	-2.521958
158	1	0	5.230734	-4.720243	-1.815601
159	6	0	2.370582	-4.207769	2.609376
160	1	0	8.000550	-1.891753	-4.273142
161	8	0	6.035173	-0.745024	-4.774455
162	6	0	2.447673	4.255289	-2.587033
163	8	0	6.085877	-3.271346	-3.842530
164	6	0	2.375517	-4.899646	1.314637
165	6	0	4.795748	-1.309236	-4.477251
166	6	0	4.822171	-2.698340	-4.031200
167	6	0	2.389968	-1.331288	-4.401124
168	6	0	2.410618	-2.746480	-4.002072
169	6	0	3.680261	3.833915	-3.195655
170	6	0	3.733820	5.236306	-0.667178
171	6	0	3.646268	3.364362	3.745235
172	6	0	3.603947	0.666361	4.788937
173	6	0	3.622422	-0.641624	-4.670336
174	6	0	3.676760	-3.413662	-3.834108
175	6	0	3.612608	-3.805309	3.212369
176	6	0	3.629340	-5.134801	0.643706
177	1	0	3.662642	3.388011	-4.182551
178	1	0	3.764476	5.811583	0.250384
179	1	0	3.592916	0.368530	-5.058407
180	1	0	3.666950	4.394213	3.409967
181	1	0	3.702442	-4.462951	-3.566315
182	1	0	3.585067	-0.314073	5.248110
183	1	0	3.608847	-3.383230	4.209798
184	1	0	3.649853	-5.691326	-0.285911
185	7	0	1.218453	-3.287028	-3.769234
186	7	0	1.182203	-0.788064	-4.479717
187	7	0	1.172698	-5.255244	0.862247
188	7	0	1.168510	-4.018754	3.148575
189	7	0	1.156454	0.811068	4.659325
190	7	0	1.185652	3.239659	3.745918
191	7	0	1.275485	5.332927	-0.835993
192	7	0	1.232731	4.042528	-3.093580
193	1	0	9.231490	0.725695	-1.875918
194	1	0	9.111543	1.824526	0.688323
195	1	0	9.155227	-0.717018	1.843669
196	1	0	9.068883	-1.817330	-0.681191
197	6	0	9.858856	-1.507270	-3.268055
198	1	0	10.259884	-0.887257	-4.075914
199	6	0	9.827339	-3.319798	1.454066
200	1	0	10.241371	-2.402320	1.022969
201	1	0	10.200958	-4.160513	0.861539
202	6	0	9.835879	1.478015	3.287152
203	1	0	10.252015	1.079606	2.355899
204	1	0	10.213163	0.861407	4.108876
205	6	0	9.905547	3.309588	-1.448325
206	1	0	10.304242	2.391316	-1.004590
207	1	0	10.283880	4.150772	-0.859602
208	1	0	10.215954	-3.411505	2.473032
209	1	0	10.267502	-1.128973	-2.325209
210	1	0	10.218708	2.495669	3.410757
211	1	0	10.305158	3.387582	-2.464252
212	1	0	10.225143	-2.529984	-3.399153
213	34	0	-0.069841	4.793665	-2.002781
214	34	0	-0.173840	2.035061	4.197221
215	34	0	-0.145319	-2.043761	-4.088994
216	34	0	-0.155964	-4.746300	2.068646
217	6	0	5.478607	0.157259	0.088690
218	6	0	4.312796	-0.300406	-0.805142
219	1	0	6.380578	0.360899	-0.502064
220	1	0	5.220598	1.074484	0.637597
221	1	0	5.729628	-0.618896	0.826178
222	6	0	3.073710	-0.669612	0.035909
223	1	0	4.057468	0.493068	-1.524021
224	1	0	4.627288	-1.175314	-1.396988
225	1	0	3.334502	-1.488557	0.722207
226	1	0	2.772067	0.186700	0.653363
227	6	0	1.905599	-1.092606	-0.848734
228	1	0	2.151937	-1.954713	-1.475793
229	1	0	1.510986	-0.268475	-1.450806
230	35	0	0.350848	-1.710481	0.283153
231	6	0	-2.108533	1.030900	-0.973233
232	1	0	-2.403385	1.838347	-1.647278
233	1	0	-1.717832	0.175573	-1.531960
234	6	0	-3.223362	0.652505	-0.006733
235	6	0	-4.493707	0.231181	-0.774666
236	1	0	-3.461070	1.509394	0.639907
237	1	0	-2.888697	-0.164850	0.645014
238	6	0	-5.614011	-0.185708	0.192249
239	1	0	-4.840549	1.073104	-1.395512
240	1	0	-4.263619	-0.596731	-1.462082
241	1	0	-6.545150	-0.402005	-0.345811
242	1	0	-5.334385	-1.085101	0.759494
243	1	0	-5.821797	0.618280	0.912337
244	35	0	-0.516121	1.783515	0.029506

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Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.307222	1.912852	-3.083397
2	6	0	-7.698981	2.664214	-1.899891
3	6	0	-7.727094	0.502093	-3.166669
4	1	0	-7.986094	2.438614	-3.986557
5	6	0	-8.209077	2.532211	-0.598091
6	6	0	-6.608196	3.532315	-2.070728
7	6	0	-8.302082	-0.614529	-2.535229
8	6	0	-6.560437	0.285802	-3.915716
9	6	0	-7.699896	3.234593	0.506861

10	6	0	-6.060906	4.239172	-1.001168
11	8	0	-6.082056	3.763044	-3.369914
12	6	0	-7.747146	-1.903787	-2.619894
13	6	0	-5.997416	-0.979813	-4.058964
14	8	0	-6.014002	1.377738	-4.627271
15	6	0	-8.319674	3.097392	1.897218
16	6	0	-6.601546	4.079867	0.274355
17	1	0	-5.253598	4.943869	-1.164927
18	6	0	-4.814804	3.229763	-3.635042
19	6	0	-8.345831	-3.123674	-1.921093
20	6	0	-6.581495	-2.052120	-3.387688
21	1	0	-5.155792	-1.138616	-4.720237
22	6	0	-4.779524	1.909356	-4.255815
23	1	0	-7.999652	3.970926	2.471374
24	6	0	-7.744101	1.871209	2.601236
25	8	0	-6.078011	4.875749	1.325488
26	6	0	-7.744879	-3.267924	-0.523085
27	1	0	-8.027676	-4.000501	-2.491439
28	8	0	-6.057117	-3.350636	-3.570009
29	6	0	-8.311752	0.587458	2.524196
30	6	0	-6.567869	2.012889	3.353633
31	6	0	-4.813602	4.545173	1.832158
32	6	0	-2.401189	3.304445	-3.624144
33	6	0	-8.263107	-2.580450	0.587187
34	6	0	-6.635441	-4.099719	-0.297920
35	6	0	-4.816421	-3.695230	-3.028881
36	6	0	-2.372450	1.950578	-4.197668
37	6	0	-7.742230	-0.532201	3.156821
38	6	0	-5.990057	0.940313	4.027319
39	8	0	-6.035693	3.310206	3.512730
40	6	0	-4.789884	3.652461	2.986502
41	6	0	-7.733533	-2.695435	1.883418
42	6	0	-6.081606	-4.250193	0.971894
43	8	0	-6.117452	-4.886564	-1.358398
44	6	0	-4.849643	-4.565541	-1.860545
45	6	0	-8.329359	-1.941249	3.073343
46	6	0	-6.572543	-0.319361	3.902609
47	1	0	-5.137840	1.091084	4.676488
48	6	0	-2.405543	4.746387	1.922384
49	6	0	-6.623965	-3.542365	2.043554
50	1	0	-5.264562	-4.943634	1.133003
51	6	0	-2.410206	-3.834512	-3.066062
52	1	0	-8.002727	-2.470359	3.972788
53	8	0	-6.036269	-1.403445	4.631670
54	6	0	-2.384806	3.803747	3.049518
55	8	0	-6.078893	-3.759188	3.335032
56	6	0	-2.441860	-4.749755	-1.919635
57	6	0	-4.792385	-1.927004	4.275969
58	6	0	-4.813993	-3.220535	3.603799
59	6	0	-2.384407	-1.960436	4.269602
60	6	0	-2.400128	-3.280612	3.625576
61	6	0	-3.617322	3.285653	3.580762
62	6	0	-3.670779	5.094823	1.322517
63	6	0	-3.674001	3.928596	-3.361109
64	6	0	-3.600315	1.285685	-4.540351
65	6	0	-3.621317	-1.313955	4.613024
66	6	0	-3.664182	-3.896641	3.309098
67	6	0	-3.639077	-3.336283	-3.621075
68	6	0	-3.708960	-5.101251	-1.331397
69	1	0	-3.594951	2.681244	4.478941
70	1	0	-3.705860	5.813606	0.512277
71	1	0	-3.599167	-0.387283	5.172523
72	1	0	-3.709832	4.934156	-2.959470
73	1	0	-3.687304	-4.887246	2.870957
74	1	0	-3.563703	0.334191	-5.055581
75	1	0	-3.612748	-2.748667	-4.530428
76	1	0	-3.745969	-5.805193	-0.508599
77	7	0	-1.198306	-3.788490	3.355783
78	7	0	-1.176094	-1.450617	4.486253
79	7	0	-1.246618	-5.169832	-1.495898
80	7	0	-1.192892	-3.539782	-3.522691
81	7	0	-1.162023	1.429259	-4.348593
82	7	0	-1.210240	3.820633	-3.331362
83	7	0	-1.210649	5.193593	1.536460
84	7	0	-1.177901	3.511799	3.523371
85	1	0	-9.228676	0.456198	1.957030
86	1	0	-9.050258	1.863067	-0.439586
87	1	0	-9.215083	-0.477154	-1.963047
88	1	0	-9.117694	-1.926721	0.435811
89	6	0	-9.867628	-1.938048	3.049227
90	1	0	-10.243150	-2.965772	3.043201
91	1	0	-10.281257	-1.430839	2.171283
92	6	0	-9.883799	-3.096553	-1.898296
93	1	0	-10.289556	-2.249407	-1.335503
94	1	0	-10.265910	-4.011885	-1.436381
95	6	0	-9.845490	1.918247	-3.047588
96	1	0	-10.255381	1.419434	-2.163174
97	1	0	-10.242406	1.407792	-3.930598
98	6	0	-9.857423	3.088959	1.851916
99	1	0	-10.265218	2.243966	1.287366
100	1	0	-10.222490	4.006641	1.380890
101	1	0	-10.272593	-3.033043	-2.919378
102	1	0	-10.214563	2.948300	-3.045324
103	1	0	-10.255071	-1.430737	3.938248
104	1	0	-10.260964	3.034638	2.867814
105	34	0	0.105326	-4.450526	-2.555673
106	34	0	0.154286	-2.630303	3.934410
107	34	0	0.158616	2.634203	-3.810292
108	34	0	0.134346	4.448568	2.598724
109	6	0	8.370732	0.841378	3.523026
110	6	0	7.782303	1.935844	2.631575
111	6	0	7.787830	-0.524880	3.161770
112	1	0	8.039800	1.060497	4.541898
113	6	0	8.321679	2.250648	1.373075
114	6	0	6.669796	2.683794	3.051629
115	6	0	8.350836	-1.375633	2.194721
116	6	0	6.635976	-0.981452	3.822514
117	6	0	7.811052	3.267543	0.547683
118	6	0	6.134832	3.705518	2.268942
119	8	0	6.110686	2.449964	4.331996
120	6	0	7.801596	-2.629216	1.872567
121	6	0	6.069244	-2.224145	3.547450

122	8	0	6.093560	-0.193314	4.862276
123	6	0	8.421498	3.596107	-0.814525
124	6	0	6.697969	3.979734	1.023978
125	1	0	5.316368	4.309168	2.641808
126	6	0	4.851097	1.833583	4.382769
127	6	0	8.386907	-3.548861	0.804117
128	6	0	6.644499	-3.023187	2.562756
129	1	0	5.224644	-2.583388	4.120629
130	6	0	4.842193	0.401657	4.664158
131	1	0	8.106447	4.613319	-1.062328
132	6	0	7.824075	2.678692	-1.879099
133	8	0	6.186627	5.070335	0.277636
134	6	0	7.775623	-3.209857	-0.554610
135	1	0	8.063207	-4.563883	1.049544
136	8	0	6.118321	-4.312502	2.323504
137	6	0	8.369534	1.426594	-2.210673
138	6	0	6.664615	3.078231	-2.564115
139	6	0	4.922850	4.943755	-0.317862
140	6	0	2.426669	1.847491	4.312870
141	6	0	8.296960	-2.197011	-1.377678
142	6	0	6.653595	-3.908794	-1.030701
143	6	0	4.862951	-4.467178	1.725898
144	6	0	2.420584	0.387443	4.596461
145	6	0	7.793472	0.575574	-3.170832
146	6	0	6.081442	2.282775	-3.546820
147	8	0	6.151460	4.371315	-2.325488
148	6	0	4.902174	4.539519	-1.719198
149	6	0	7.766242	-1.881138	-2.639962
150	6	0	6.100456	-3.634877	-2.280162
151	8	0	6.127510	-4.991309	-0.284428
152	6	0	4.868208	-4.858142	0.317683
153	6	0	8.367641	-0.794162	-3.532203
154	6	0	6.637461	1.034788	-3.820772
155	1	0	5.240223	2.649044	-4.120514
156	6	0	2.507269	5.185779	-0.338260
157	6	0	6.654357	-2.625899	-3.066165
158	1	0	5.278355	-4.232989	-2.654097
159	6	0	2.446052	-4.674955	1.784829
160	1	0	8.037745	-1.010977	-4.551875
161	8	0	6.082834	0.244429	-4.853510
162	6	0	2.486779	4.752047	-1.757536
163	8	0	6.116928	-2.404229	-4.359902
164	6	0	2.449892	-5.100770	0.358625
165	6	0	4.837124	-0.356924	-4.650650
166	6	0	4.854308	-1.798904	-4.419966
167	6	0	2.418092	-0.360013	-4.550713
168	6	0	2.431123	-1.834704	-4.344784
169	6	0	3.733853	4.447005	-2.417870
170	6	0	3.776778	5.268383	0.348242
171	6	0	3.694673	2.538177	4.231010
172	6	0	3.678765	-0.295560	4.785943
173	6	0	3.669359	0.338448	-4.729240
174	6	0	3.704426	-2.519648	-4.300964
175	6	0	3.702611	-4.377143	2.435414
176	6	0	3.715951	-5.171510	-0.342021
177	1	0	3.719369	4.211366	-3.475136
178	1	0	3.800191	5.628356	1.369968
179	1	0	3.644567	1.397843	-4.951176
180	1	0	3.697466	3.609983	4.073908
181	1	0	3.715864	-3.596287	-4.183130
182	1	0	3.664776	-1.345111	5.052017
183	1	0	3.698341	-4.149941	3.494599
184	1	0	3.730002	-5.522017	-1.367368
185	7	0	1.261187	-2.427761	-4.173084
186	7	0	1.238242	0.232764	-4.546905
187	7	0	1.275664	-5.393431	-0.184266
188	7	0	1.270638	-4.612439	2.392709
189	7	0	1.241129	-0.207931	4.654444
190	7	0	1.249767	2.427845	4.139376
191	7	0	1.334578	5.470024	0.223650
192	7	0	1.298022	4.684139	-2.350120
193	1	0	9.279255	1.105995	-1.710907
194	1	0	9.175065	1.678231	1.019480
195	1	0	9.251965	-1.054375	1.680110
196	1	0	9.158449	-1.637261	-1.023808
197	6	0	9.906018	-0.811446	-3.510577
198	1	0	10.298603	-0.058035	-4.200625
199	6	0	9.924606	-3.525764	0.778685
200	1	0	10.334156	-2.539400	0.537057
201	1	0	10.296690	-4.230263	0.028420
202	6	0	9.909484	0.844386	3.505833
203	1	0	10.326142	0.635603	2.514852
204	1	0	10.292716	0.083814	4.193335
205	6	0	9.958967	3.558544	-0.792952
206	1	0	10.359673	2.570573	-0.543117
207	1	0	10.338920	4.265543	-0.049110
208	52	0	-0.172366	5.249916	-1.096400
209	52	0	-0.274963	1.104989	4.362247
210	52	0	-0.274143	-1.100266	-4.305126
211	52	0	-0.226351	-5.161395	1.154122
212	1	0	10.318906	-3.817056	1.757242
213	1	0	10.322108	-0.602318	-2.519430
214	1	0	10.284933	1.822430	3.822120
215	1	0	10.354368	3.838259	-1.774505
216	1	0	10.272709	-1.794717	-3.820885
217	6	0	5.801491	0.016252	0.198239
218	6	0	4.591005	0.033525	-0.747917
219	1	0	6.728323	0.306671	-0.310553
220	1	0	5.654696	0.703513	1.042805
221	1	0	5.948880	-0.993207	0.606776
222	6	0	3.364992	-0.583058	-0.045658
223	1	0	4.373096	1.061753	-1.071924
224	1	0	4.820243	-0.545587	-1.656513
225	1	0	3.594146	-1.630092	0.201056
226	1	0	3.182139	-0.064457	0.905156
227	6	0	2.113278	-0.519909	-0.918634
228	1	0	2.263117	-0.999947	-1.888860
229	1	0	1.725966	0.494263	-1.048361
230	53	0	0.486465	-1.648576	0.013446
231	6	0	-2.247477	1.221730	-0.793964
232	1	0	-2.557323	2.093334	-1.376163
233	1	0	-1.827745	0.445785	-1.441253

234	6	0	-3.367193	0.709907	0.101518
235	6	0	-4.613043	0.326988	-0.719657
236	1	0	-3.643503	1.489120	0.827649
237	1	0	-3.013623	-0.156523	0.676287
238	6	0	-5.736441	-0.160621	0.207225
239	1	0	-4.962721	1.206180	-1.285388
240	1	0	-4.360047	-0.447415	-1.459084
241	1	0	-6.665573	-0.345474	-0.344022
242	1	0	-5.454900	-1.092189	0.719208
243	1	0	-5.941121	0.601730	0.971120
244	35	0	-0.704269	1.871919	0.330621

RI-RBr**@A_{Se}+A_{Te}**

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.324415	1.053913	-3.502725
2	6	0	-7.722035	2.080421	-2.543128
3	6	0	-7.756314	-0.337335	-3.226147
4	1	0	-7.991941	1.333394	-4.506103
5	6	0	-8.246687	2.295098	-1.257837
6	6	0	-6.622233	2.868219	-2.919816
7	6	0	-8.339811	-1.252296	-2.332668
8	6	0	-6.592749	-0.748101	-3.895444
9	6	0	-7.739311	3.256520	-0.368325
10	6	0	-6.077235	3.825332	-2.064162
11	8	0	-6.078839	2.743000	-4.224607
12	6	0	-7.797316	-2.526248	-2.085072
13	6	0	-6.040297	-2.012404	-3.707023
14	8	0	-6.034689	0.120017	-4.860022
15	6	0	-8.368777	3.493370	1.003103
16	6	0	-6.629285	4.004816	-0.796636
17	1	0	-5.261687	4.457161	-2.395898
18	6	0	-4.815144	2.142136	-4.316794
19	6	0	-8.404858	-3.513559	-1.089620
20	6	0	-6.633472	-2.876348	-2.788335
21	1	0	-5.193621	-2.339030	-4.296507
22	6	0	-4.793082	0.711809	-4.613594
23	1	0	-8.049972	4.487624	1.327128
24	6	0	-7.798150	2.498390	2.008953
25	8	0	-6.116602	5.042214	0.020606
26	6	0	-7.811606	-3.279213	0.299737
27	1	0	-8.085613	-4.511395	-1.402545
28	8	0	-6.116240	-4.182557	-2.642530
29	6	0	-8.359340	1.233186	2.253279
30	6	0	-6.639345	2.840247	2.723231
31	6	0	-4.860038	4.871614	0.622395
32	6	0	-2.391244	2.181791	-4.234581
33	6	0	-8.339127	-2.330909	1.193271
34	6	0	-6.693631	-4.011319	0.731431
35	6	0	-4.870336	-4.381873	-2.036869
36	6	0	-2.373853	0.718258	-4.505383
37	6	0	-7.806791	0.319887	3.168370
38	6	0	-6.075017	1.979173	3.660809
39	8	0	-6.114690	4.140302	2.563461
40	6	0	-4.858101	4.346134	1.985900
41	6	0	-7.805763	-2.096597	2.472208
42	6	0	-6.141396	-3.823190	1.996944
43	8	0	-6.167898	-5.039058	-0.089228
44	6	0	-4.899445	-4.865680	-0.660613
45	6	0	-8.398600	-1.064714	3.433276
46	6	0	-6.654594	0.727043	3.859541
47	1	0	-5.231535	2.296163	4.259812
48	6	0	-2.443253	5.130266	0.700533
49	6	0	-6.689464	-2.863515	2.846087
50	1	0	-5.320412	-4.445450	2.331733
51	6	0	-2.452547	-4.573929	-2.066475
52	1	0	-8.075749	-1.354048	4.437184
53	8	0	-6.122713	-0.124866	4.853250
54	6	0	-2.443204	4.546581	2.069475
55	8	0	-6.146224	-2.724573	4.146595
56	6	0	-2.481401	-5.083369	-0.671156
57	6	0	-4.871995	-0.712351	4.630881
58	6	0	-4.883652	-2.124450	4.263051
59	6	0	-2.450270	-0.711246	4.606663
60	6	0	-2.458034	-2.155224	4.250982
61	6	0	-3.699573	4.186141	2.685152
62	6	0	-3.707784	5.263350	0.005430
63	6	0	-3.667359	2.860730	-4.166544
64	6	0	-3.622601	0.025091	-4.719467
65	6	0	-3.707036	-0.030721	4.810869
66	6	0	-3.728836	-2.829354	4.099214
67	6	0	-3.697764	-4.242421	-2.719523
68	6	0	-3.756867	-5.216574	-0.002786
69	1	0	-3.696349	3.853602	3.716048
70	1	0	-3.721624	5.713512	-0.980416
71	1	0	-3.690818	1.001015	5.138999
72	1	0	-3.684772	3.931054	-3.999912
73	1	0	-3.736298	-3.890575	3.881661
74	1	0	-3.592381	-1.022694	-4.990865
75	1	0	-3.677035	-3.948475	-3.761997
76	1	0	-3.785594	-5.634804	0.996312
77	7	0	-1.279915	-2.735312	4.076897
78	7	0	-1.269399	-0.124352	4.714207
79	7	0	-1.312734	-5.387645	-0.115330
80	7	0	-1.261315	-4.467287	-2.644392
81	7	0	-1.193363	0.127576	-4.523602
82	7	0	-1.225424	2.767462	-4.019577
83	7	0	-1.267932	5.481451	0.195478
84	7	0	-1.269377	4.404783	2.664905
85	1	0	-9.256159	0.949126	1.710144
86	1	0	-9.096958	1.697306	-0.941211
87	1	0	-9.248046	-0.963872	-1.811081
88	1	0	-9.201124	-1.748766	0.878837
89	6	0	-9.937107	-1.059909	3.404900
90	1	0	-10.318477	-2.055813	3.650874
91	1	0	-10.345848	-0.781978	2.427653
92	6	0	-9.942624	-3.478489	-1.085229
93	1	0	-10.348238	-2.509251	-0.776510

94	1	0	-10.331149	-4.233215	-0.394498
95	6	0	-9.863064	1.075672	-3.483150
96	1	0	-10.282136	0.814689	-2.505638
97	1	0	-10.256876	0.362363	-4.214089
98	6	0	-9.906169	3.473104	0.953463
99	1	0	-10.312124	2.508109	0.632220
100	1	0	-10.267418	4.232458	0.253022
101	52	0	0.207579	-5.087979	-1.409716
102	52	0	0.243931	-1.430165	4.396636
103	52	0	0.313673	1.449846	-4.201359
104	52	0	0.231108	5.073262	1.495802
105	1	0	-10.324868	-3.693043	-2.088219
106	1	0	-10.225325	2.075733	-3.740611
107	1	0	-10.322739	-0.346456	4.139953
108	1	0	-10.314478	3.690404	1.945530
109	6	0	8.297917	1.743408	3.218240
110	6	0	7.717960	2.572103	2.072153
111	6	0	7.706079	0.334991	3.210559
112	1	0	7.965116	2.217510	4.145530
113	6	0	8.262854	2.547339	0.777597
114	6	0	6.606807	3.405923	2.279076
115	6	0	8.264358	-0.731880	2.485406
116	6	0	6.548467	0.066052	3.956802
117	6	0	7.760037	3.315014	-0.286553
118	6	0	6.084042	4.197004	1.257230
119	8	0	6.048277	3.521139	3.577149
120	6	0	7.705404	-2.021150	2.480233
121	6	0	5.972584	-1.202484	3.997975
122	8	0	6.008946	1.094995	4.761937
123	6	0	8.375308	3.260079	-1.685020
124	6	0	6.654634	4.138091	-0.013459
125	1	0	5.269410	4.882885	1.458064
126	6	0	4.786625	2.956637	3.802121
127	6	0	8.291747	-3.189947	1.693965
128	6	0	6.544408	-2.222945	3.241957
129	1	0	5.129585	-1.404607	4.645840
130	6	0	4.766488	1.636851	4.422245
131	1	0	8.064655	4.172797	-2.200706
132	6	0	7.780074	2.089337	-2.467023
133	8	0	6.151962	5.005369	-1.017260
134	6	0	7.690599	-3.230639	0.290390
135	1	0	7.968480	-4.103543	2.199923
136	8	0	6.019147	-3.531561	3.328571
137	6	0	8.336288	0.797669	-2.475504
138	6	0	6.614107	2.291057	-3.222447
139	6	0	4.885403	4.727076	-1.548416
140	6	0	2.372618	2.995273	3.794583
141	6	0	8.216036	-2.466483	-0.763283
142	6	0	6.592090	-4.056684	-0.004085
143	6	0	4.775504	-3.837450	2.773613
144	6	0	2.357020	1.653368	4.392795
145	6	0	7.760740	-0.271336	-3.184635
146	6	0	6.031896	1.270287	-3.971228
147	8	0	6.094582	3.600206	-3.311595
148	6	0	4.852123	3.918096	-2.760063
149	6	0	7.718601	-2.517181	-2.076460
150	6	0	6.071495	-4.144976	-1.293718
151	8	0	6.057003	-4.900791	1.000644
152	6	0	4.795649	-4.603112	1.531557
153	6	0	8.336624	-1.686462	-3.200355
154	6	0	6.595413	-0.002343	-3.918248
155	1	0	5.192672	1.476441	-4.622353
156	6	0	2.480208	4.938109	-1.614947
157	6	0	6.631196	-3.373110	-2.312009
158	1	0	5.266073	-4.836952	-1.510989
159	6	0	2.370856	-4.008389	2.840856
160	1	0	8.018946	-2.145155	-4.140466
161	8	0	6.052426	-1.041494	-4.706371
162	6	0	2.448420	4.081711	-2.805074
163	8	0	6.109383	-3.514614	-3.625503
164	6	0	2.388437	-4.811534	1.611635
165	6	0	4.815338	-1.595427	-4.379156
166	6	0	4.844577	-2.955386	-3.851758
167	6	0	2.408297	-1.629408	-4.325652
168	6	0	2.431270	-3.016021	-3.839969
169	6	0	3.675653	3.599663	-3.376843
170	6	0	3.746149	5.246667	-1.000609
171	6	0	3.634818	3.633000	3.518098
172	6	0	3.596356	1.004024	4.724104
173	6	0	3.638954	-0.949537	-4.623613
174	6	0	3.699993	-3.664223	-3.622996
175	6	0	3.605967	-3.545447	3.414364
176	6	0	3.648748	-5.090431	0.969330
177	1	0	3.650272	3.060006	-4.315468
178	1	0	3.782731	5.905208	-0.141050
179	1	0	3.606785	0.035250	-5.072278
180	1	0	3.654452	4.639506	3.117951
181	1	0	3.730289	-4.695961	-3.294015
182	1	0	3.577851	0.053801	5.242826
183	1	0	3.591704	-3.041104	4.372800
184	1	0	3.678919	-5.721901	0.089212
185	7	0	1.237884	-3.545586	-3.581149
186	7	0	1.200274	-1.091286	-4.440833
187	7	0	1.192404	-5.222083	1.187346
188	7	0	1.164987	-3.787098	3.358859
189	7	0	1.149683	1.130689	4.578619
190	7	0	1.172708	3.505029	3.528384
191	7	0	1.285931	5.347475	-1.176311
192	7	0	1.230820	3.823096	-3.283474
193	1	0	9.251953	0.619847	-1.918962
194	1	0	9.116956	1.902554	0.589628
195	1	0	9.166928	-0.552552	1.908389
196	1	0	9.058622	-1.812536	-0.556393
197	6	0	9.874673	-1.700168	-3.155786
198	1	0	10.278723	-1.128206	-3.997013
199	6	0	9.830107	-3.173820	1.669298
200	1	0	10.241838	-2.288244	1.173976
201	1	0	10.204616	-4.053633	1.137148
202	6	0	9.836777	1.733758	3.209501
203	1	0	10.257101	1.276457	2.307600
204	1	0	10.212301	1.172797	4.070992
205	6	0	9.912708	3.227081	-1.648183

206	1	0	10.310858	2.343971	-1.137497
207	1	0	10.291915	4.109469	-1.123791
208	34	0	-0.062394	4.695273	-2.278443
209	34	0	-0.182396	2.323513	4.049072
210	34	0	-0.123401	-2.322687	-3.979995
211	34	0	-0.145937	-4.620309	2.339597
212	1	0	10.220207	-3.192753	2.691709
213	1	0	10.280760	-1.268160	-2.235114
214	1	0	10.217101	2.758173	3.267762
215	1	0	10.312136	3.229030	-2.667237
216	1	0	10.240513	-2.728968	-3.226250
217	6	0	5.663294	0.281518	0.148469
218	6	0	4.628697	-0.424898	-0.740584
219	1	0	6.650790	0.315402	-0.326936
220	1	0	5.355808	1.315792	0.361406
221	1	0	5.774139	-0.243304	1.108047
222	6	0	3.295701	-0.608966	0.010936
223	1	0	4.463342	0.159056	-1.658766
224	1	0	5.014697	-1.408200	-1.052429
225	1	0	3.463319	-1.246517	0.891486
226	1	0	2.944096	0.363148	0.380893
227	6	0	2.228883	-1.232769	-0.886896
228	1	0	2.527656	-2.219458	-1.254667
229	1	0	1.955891	-0.580558	-1.721596
230	53	0	0.378151	-1.566299	0.221222
231	6	0	-2.361935	1.133058	-1.014044
232	1	0	-2.708280	1.916269	-1.691836
233	1	0	-1.926271	0.297232	-1.570030
234	6	0	-3.448621	0.702937	-0.039482
235	6	0	-4.678472	0.162604	-0.793537
236	1	0	-3.751904	1.561957	0.576702
237	1	0	-3.060546	-0.064237	0.643851
238	6	0	-5.790277	-0.228167	0.190138
239	1	0	-5.054759	0.936040	-1.482439
240	1	0	-4.395077	-0.702546	-1.411632
241	1	0	-6.698587	-0.539082	-0.337508
242	1	0	-5.474546	-1.057380	0.839247
243	1	0	-6.052725	0.625897	0.829027
244	35	0	-0.816137	1.972832	-0.020282

RI-RI@A_{Se}+A_{Te}

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	-8.371634	-3.668011	0.069079
2	6	0	-7.765392	-3.030599	-1.179441
3	6	0	-7.777619	-3.010816	1.311328
4	1	0	-8.047962	-4.712342	0.077997
5	6	0	-8.300123	-1.873317	-1.771180
6	6	0	-6.628072	-3.595111	-1.781089
7	6	0	-8.315536	-1.847106	1.886199
8	6	0	-6.625466	-3.552159	1.904092
9	6	0	-7.767120	-1.286277	-2.932335
10	6	0	-6.076872	-3.057196	-2.941822
11	8	0	-6.104397	-4.807568	-1.275529
12	6	0	-7.753260	-1.217562	3.010277
13	6	0	-6.047036	-2.973884	3.029972
14	8	0	-6.111121	-4.776103	1.418567
15	6	0	-8.382540	-0.046653	-3.587784
16	6	0	-6.644198	-1.911425	-3.498802
17	1	0	-5.248562	-3.554356	-3.431364
18	6	0	-4.848939	-4.838224	-0.654061
19	6	0	-8.348061	0.045986	3.635502
20	6	0	-6.606343	-1.812371	3.560676
21	1	0	-5.200336	-3.445133	3.512860
22	6	0	-4.851970	-4.824130	0.807537
23	1	0	-8.048826	-0.051890	-4.629205
24	6	0	-7.835734	1.239033	-2.964789
25	8	0	-6.102792	-1.411561	-4.710092
26	6	0	-7.798140	1.308755	2.967240
27	1	0	-7.999763	0.070250	4.672027
28	8	0	-6.040086	-1.269970	4.738757
29	6	0	-8.429605	1.874564	-1.859606
30	6	0	-6.686364	1.840273	-3.503274
31	6	0	-4.848934	-0.790892	-4.622570
32	6	0	-2.438013	-5.141933	-0.656827
33	6	0	-8.386296	1.901400	1.835711
34	6	0	-6.655709	1.935837	3.491914
35	6	0	-4.790113	-0.647874	4.617945
36	6	0	-2.440471	-5.124799	0.831258
37	6	0	-7.908526	3.043079	-1.274844
38	6	0	-6.160892	3.021661	-2.984434
39	8	0	-6.105673	1.280518	-4.664468
40	6	0	-4.851551	0.668144	-4.566564
41	6	0	-7.881472	3.064891	1.225707
42	6	0	-6.137300	3.103810	2.937348
43	8	0	-6.061500	1.417665	4.666224
44	6	0	-4.802567	0.811239	4.564369
45	6	0	-8.511186	3.685114	-0.024233
46	6	0	-6.760539	3.597225	-1.866022
47	1	0	-5.323318	3.509429	-3.466520
48	6	0	-2.428237	-0.814285	-4.489087
49	6	0	-6.741853	3.646487	1.805317
50	1	0	-5.302078	3.609658	3.405011
51	6	0	-2.370146	-0.655613	4.477389
52	1	0	-8.213306	4.737228	-0.036025
53	8	0	-6.262698	4.829351	-1.383770
54	6	0	-2.433394	0.673244	-4.422704
55	8	0	-6.254446	4.876124	1.300986
56	6	0	-2.382942	0.833500	4.423120
57	6	0	-5.001915	4.887767	-0.777731
58	6	0	-4.998408	4.918544	0.681921
59	6	0	-2.589728	5.162330	-0.802446
60	6	0	-2.586470	5.194511	0.685229
61	6	0	-3.692971	1.379028	-4.490151
62	6	0	-3.690992	-1.507779	-4.613861
63	6	0	-3.694123	-4.998922	-1.362466
64	6	0	-3.700979	-4.968576	1.525311
65	6	0	-3.850293	5.016186	-1.497370

66	6	0	-3.844279	5.079390	1.390497
67	6	0	-3.628617	-1.357597	4.594010
68	6	0	-3.648877	1.530269	4.487516
69	1	0	-3.681432	2.461864	-4.498950
70	1	0	-3.687543	-2.586782	-4.707957
71	1	0	-3.857852	5.060087	-2.579847
72	1	0	-3.699828	-5.077503	-2.443291
73	1	0	-3.848850	5.165580	2.470396
74	1	0	-3.711412	-5.020730	2.607531
75	1	0	-3.616041	-2.436523	4.685984
76	1	0	-3.645981	2.613206	4.504105
77	7	0	-1.406695	5.311487	1.284930
78	7	0	-1.412323	5.257674	-1.410691
79	7	0	-1.213196	1.435391	4.317895
80	7	0	-1.191412	-1.247544	4.412377
81	7	0	-1.267176	-5.248815	1.439368
82	7	0	-1.262850	-5.283738	-1.256864
83	7	0	-1.256378	-1.416570	-4.392291
84	7	0	-1.261296	1.265382	-4.291726
85	1	0	-9.321835	1.432437	-1.425255
86	1	0	-9.173635	-1.416226	-1.314549
87	1	0	-9.204766	-1.412367	1.438361
88	1	0	-9.270016	1.435396	1.408588
89	6	0	-10.047396	3.617504	-0.005894
90	1	0	-10.433307	4.126683	0.882687
91	1	0	-10.430872	2.591874	0.009063
92	6	0	-9.886755	0.018636	3.645523
93	1	0	-10.319831	-0.003680	2.639881
94	1	0	-10.273381	0.908417	4.152231
95	6	0	-9.909348	-3.640144	0.058810
96	1	0	-10.320028	-2.625098	0.050942
97	1	0	-10.297402	-4.146537	0.948146
98	6	0	-9.920951	-0.092528	-3.576750
99	1	0	-10.341043	-0.099146	-2.565447
100	1	0	-10.270914	-0.996346	-4.085078
101	1	0	-10.241855	-0.869132	4.178072
102	1	0	-10.286804	-4.156076	-0.829590
103	1	0	-10.454216	4.109758	-0.894778
104	1	0	-10.325510	0.780696	-4.098124
105	52	0	0.324268	0.107288	4.305285
106	52	0	0.085508	5.452360	-0.068656
107	52	0	0.229534	-5.436676	0.093475
108	52	0	0.268558	-0.071275	-4.250233
109	6	0	8.325565	2.568375	-2.648970
110	6	0	7.757050	1.192588	-3.000804
111	6	0	7.717177	3.074147	-1.338513
112	1	0	7.992657	3.254894	-3.432572
113	6	0	8.354551	-0.028660	-2.638095
114	6	0	6.551121	1.128935	-3.716612
115	6	0	8.240590	2.690255	-0.092318
116	6	0	6.613480	3.944544	-1.318486
117	6	0	7.782760	-1.276779	-2.950926
118	6	0	5.973232	-0.081284	-4.088163
119	8	0	5.983046	2.340969	-4.155399
120	6	0	7.731669	3.134979	1.140060
121	6	0	6.072055	4.406263	-0.120632
122	8	0	6.058035	4.450666	-2.524968
123	6	0	8.388367	-2.625045	-2.548817
124	6	0	6.583341	-1.264866	-3.679949
125	1	0	5.104579	-0.103697	-4.731517
126	6	0	4.743572	2.778042	-3.693832
127	6	0	8.350440	2.685623	2.465176
128	6	0	6.622610	3.997327	1.092150
129	1	0	5.251069	5.114227	-0.132476
130	6	0	4.782141	3.979750	-2.867840
131	1	0	8.063520	-3.349456	-3.301032
132	6	0	7.804462	-3.090850	-1.212632
133	8	0	6.053231	-2.499961	-4.106376
134	6	0	7.784105	1.324873	2.873976
135	1	0	8.022459	3.402403	3.223197
136	8	0	6.073660	4.549843	2.280199
137	6	0	8.341701	-2.665541	0.015296
138	6	0	6.692662	-3.948717	-1.151775
139	6	0	4.815074	-2.942596	-3.643989
140	6	0	2.337525	2.831793	-3.648920
141	6	0	8.377138	0.090523	2.550820
142	6	0	6.587070	1.290221	3.606168
143	6	0	4.804481	4.092617	2.663857
144	6	0	2.366754	4.082131	-2.874884
145	6	0	7.819183	-3.035399	1.266888
146	6	0	6.156385	-4.361951	0.066752
147	8	0	6.137676	-4.499390	-2.336836
148	6	0	4.860356	-4.066117	-2.717262
149	6	0	7.811848	-1.144284	2.921753
150	6	0	6.014220	0.095278	4.031449
151	8	0	6.029753	2.518540	4.014833
152	6	0	4.782775	2.941499	3.558610
153	6	0	8.417605	-2.507830	2.573297
154	6	0	6.707972	-3.897088	1.258708
155	1	0	5.337746	-5.072249	0.085572
156	6	0	2.408882	-3.037588	-3.642995
157	6	0	6.621922	-1.103323	3.665307
158	1	0	5.152906	0.098744	4.685042
159	6	0	2.388605	4.202860	2.722235
160	1	0	8.104770	-3.198123	3.361776
161	8	0	6.172274	-4.395602	2.474921
162	6	0	2.448106	-4.203641	-2.751106
163	8	0	6.102266	-2.320936	4.151971
164	6	0	2.376513	3.004961	3.573858
165	6	0	4.897462	-3.951900	2.850888
166	6	0	4.860141	-2.786750	3.726818
167	6	0	2.485245	-4.087668	2.912743
168	6	0	2.455197	-2.880641	3.750728
169	6	0	3.724312	-4.701413	-2.299231
170	6	0	3.632281	-2.438613	-4.101907
171	6	0	3.562956	2.208737	-4.071648
172	6	0	3.644281	4.632325	-2.486943
173	6	0	3.758860	-4.606074	2.473225
174	6	0	3.682434	-2.262358	4.172744
175	6	0	3.657371	4.723095	2.269734
176	6	0	3.610086	2.403384	4.001793
177	1	0	3.770456	-5.579665	-1.666427

178	1	0	3.589845	-1.653627	-4.846187
179	1	0	3.798033	-5.510089	1.877233
180	1	0	3.520143	1.356210	-4.737298
181	1	0	3.646049	-1.441867	4.877796
182	1	0	3.686901	5.557865	-1.925175
183	1	0	3.688920	5.615747	1.656232
184	1	0	3.582749	1.593908	4.720051
185	7	0	1.242087	-2.440578	4.069899
186	7	0	1.287780	-4.585616	2.600397
187	7	0	1.170645	2.569919	3.920604
188	7	0	1.184249	4.694976	2.428035
189	7	0	1.171000	4.588545	-2.577124
190	7	0	1.124698	2.376541	-3.935701
191	7	0	1.190669	-2.620790	-3.979330
192	7	0	1.253415	-4.692083	-2.410049
193	1	0	9.196762	-1.995727	-0.004314
194	1	0	9.290456	-0.006691	-2.087273
195	1	0	9.082361	2.003172	-0.079160
196	1	0	9.308551	0.091507	1.991726
197	6	0	9.955120	-2.477750	2.542684
198	1	0	10.344643	-3.480173	2.341004
199	6	0	9.888112	2.699163	2.424070
200	1	0	10.302813	2.012747	1.678387
201	1	0	10.291416	2.412431	3.400431
202	6	0	9.863573	2.581936	-2.619405
203	1	0	10.282316	1.922959	-1.851575
204	1	0	10.224132	3.594803	-2.416181
205	6	0	9.926322	-2.600197	-2.537874
206	1	0	10.338388	-1.896718	-1.806845
207	1	0	10.302834	-2.311046	-3.524092
208	34	0	-0.111182	-3.716388	-3.234183
209	34	0	-0.191330	3.523721	-3.296208
210	34	0	-0.071677	-3.560121	3.379253
211	34	0	-0.158057	3.674826	3.242492
212	1	0	10.245701	3.704229	2.180753
213	1	0	10.355435	-1.807035	1.775146
214	1	0	10.259707	2.258292	-3.587146
215	1	0	10.314386	-3.593919	-2.294465
216	1	0	10.341936	-2.141386	3.509810
217	6	0	6.067693	0.007607	-0.048704
218	6	0	4.676840	-0.596536	0.163833
219	1	0	6.864494	-0.735450	0.021634
220	1	0	6.122936	0.475287	-1.039753
221	1	0	6.263150	0.788053	0.696568
222	6	0	3.647515	0.544593	0.111559
223	1	0	4.461294	-1.342138	-0.616742
224	1	0	4.619345	-1.115927	1.132568
225	1	0	3.835998	1.236873	0.945908
226	1	0	3.803402	1.117436	-0.814666
227	6	0	2.213474	0.040302	0.162627
228	1	0	1.960710	-0.456723	1.103523
229	1	0	1.960532	-0.609519	-0.678961
230	53	0	0.849720	1.731803	0.015153
231	6	0	-2.409902	-0.704718	-0.980616
232	1	0	-1.951876	0.258968	-1.225635
233	1	0	-2.587860	-1.283881	-1.890015
234	6	0	-3.652903	-0.582015	-0.107679
235	6	0	-4.791216	0.183080	-0.799013
236	1	0	-3.396936	-0.073564	0.831872
237	1	0	-4.012301	-1.585788	0.164045
238	6	0	-6.016429	0.190432	0.122788
239	1	0	-4.475256	1.210456	-1.032945
240	1	0	-5.044735	-0.299886	-1.755519
241	1	0	-6.839458	0.771603	-0.298478
242	1	0	-6.380766	-0.832960	0.281577
243	1	0	-5.762494	0.623336	1.101029
244	53	0	-0.892912	-1.820276	0.118390

RBr-RBr@A_{Te}+A_{Te}

Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	8.313323	-1.096237	-3.462960
2	6	0	7.696891	-2.115401	-2.505099
3	6	0	7.744926	0.298100	-3.198073
4	1	0	7.990967	-1.379101	-4.468767
5	6	0	8.206039	-2.323252	-1.211415
6	6	0	6.597276	-2.898960	-2.888943
7	6	0	8.326125	1.220634	-2.311581
8	6	0	6.583688	0.705852	-3.873627
9	6	0	7.670549	-3.261825	-0.314976
10	6	0	6.021576	-3.829647	-2.024203
11	8	0	6.078840	-2.799632	-4.207267
12	6	0	7.788520	2.500605	-2.083779
13	6	0	6.043709	1.979196	-3.714680
14	8	0	6.017452	-0.179516	-4.816788
15	6	0	8.278774	-3.507434	1.064600
16	6	0	6.546258	-3.987972	-0.743817
17	1	0	5.202798	-4.454935	-2.359748
18	6	0	4.810883	-2.209018	-4.313326
19	6	0	8.386859	3.487090	-1.083354
20	6	0	6.639012	2.854378	-2.808066
21	1	0	5.207847	2.306058	-4.319524
22	6	0	4.780645	-0.771400	-4.563617
23	1	0	7.947342	-4.499896	1.381370
24	6	0	7.705378	-2.511115	2.066670
25	8	0	5.993611	-4.983810	0.096871
26	6	0	7.773199	3.255986	0.297968
27	1	0	8.075891	4.485815	-1.401700
28	8	0	6.131662	4.168701	-2.694620
29	6	0	8.261742	-1.240076	2.291449
30	6	0	6.555942	-2.851191	2.796051
31	6	0	4.746987	-4.771716	0.698377
32	6	0	2.384734	-2.267578	-4.249594
33	6	0	8.284292	2.310360	1.203140
34	6	0	6.653124	3.995308	0.711599
35	6	0	4.875250	4.368915	-2.107898
36	6	0	2.366156	-0.792272	-4.442264
37	6	0	7.709090	-0.316735	3.195278

38	6	0	5.984332	-1.974195	3.714532
39	8	0	6.029670	-4.157014	2.667900
40	6	0	4.767535	-4.335032	2.090145
41	6	0	7.737041	2.092988	2.479573
42	6	0	6.091285	3.827946	1.975214
43	8	0	6.133899	5.005340	-0.133065
44	6	0	4.877163	4.816379	-0.721760
45	6	0	8.310373	1.064616	3.454308
46	6	0	6.552992	-0.713827	3.885894
47	1	0	5.142717	-2.286104	4.319350
48	6	0	2.325751	-4.938143	0.769879
49	6	0	6.627581	2.875338	2.839283
50	1	0	5.273387	4.460259	2.298147
51	6	0	2.453746	4.542384	-2.171422
52	1	0	7.980808	1.365238	4.452669
53	8	0	6.005719	0.160796	4.851319
54	6	0	2.345989	-4.489274	2.183918
55	8	0	6.075918	2.758858	4.139533
56	6	0	2.459070	4.986969	-0.757647
57	6	0	4.769189	0.760262	4.595373
58	6	0	4.805180	2.175305	4.246058
59	6	0	2.350029	0.790023	4.528718
60	6	0	2.378078	2.239691	4.208394
61	6	0	3.617150	-4.205707	2.810537
62	6	0	3.576458	-5.067766	0.057308
63	6	0	3.666932	-2.938850	-4.197707
64	6	0	3.607151	-0.081327	-4.628442
65	6	0	3.591814	0.087972	4.740153
66	6	0	3.660652	2.897610	4.082644
67	6	0	3.713912	4.247211	-2.814583
68	6	0	3.718333	5.125649	-0.067629
69	1	0	3.633863	-3.953938	3.864693
70	1	0	3.581890	-5.463015	-0.952442
71	1	0	3.568360	-0.946366	5.061492
72	1	0	3.691210	-4.015254	-4.073088
73	1	0	3.688099	3.963969	3.889947
74	1	0	3.582715	0.975361	-4.865505
75	1	0	3.714574	3.990777	-3.867882
76	1	0	3.734431	5.524702	0.940089
77	7	0	1.206963	2.826579	4.023807
78	7	0	1.152025	0.235944	4.590474
79	7	0	1.267758	5.207141	-0.213076
80	7	0	1.267261	4.428471	-2.756038
81	7	0	1.174199	-0.229722	-4.425424
82	7	0	1.218758	-2.861401	-4.073078
83	7	0	1.125016	-5.173969	0.259713
84	7	0	1.175129	-4.367419	2.789585
85	1	0	9.157958	-0.960907	1.744925
86	1	0	9.064340	-1.737482	-0.894266
87	1	0	9.228589	0.934005	-1.779296
88	1	0	9.146189	1.720666	0.903146
89	6	0	9.849069	1.044108	3.442091
90	1	0	10.237634	2.037991	3.684601
91	1	0	10.265470	0.754550	2.471544
92	6	0	9.924267	3.446225	-1.056372
93	1	0	10.321806	2.476607	-0.738615
94	1	0	10.305586	4.201767	-0.362641
95	6	0	9.851485	-1.120168	-3.427339
96	1	0	10.261070	-0.856177	-2.446692
97	1	0	10.254185	-0.410506	-4.156830
98	6	0	9.817042	-3.500917	1.035544
99	1	0	10.236007	-2.537448	0.726952
100	1	0	10.181231	-4.258726	0.335036
101	1	0	10.321800	3.656432	-2.054216
102	1	0	10.214661	-2.121649	-3.677528
103	1	0	10.219932	0.332920	4.186750
104	1	0	10.209686	-3.728718	2.031412
105	52	0	-0.260372	4.955439	-1.519421
106	52	0	-0.374744	1.550826	4.308777
107	52	0	-0.363149	-1.554012	-4.214029
108	52	0	-0.385894	-4.883266	1.592532
109	6	0	-8.342998	-1.447511	3.290991
110	6	0	-7.757203	-2.364972	2.217763
111	6	0	-7.740192	-0.046361	3.184641
112	1	0	-8.022573	-1.852081	4.255009
113	6	0	-8.287386	-2.432056	0.917629
114	6	0	-6.654059	-3.187805	2.499301
115	6	0	-8.288751	0.975205	2.389953
116	6	0	-6.581292	0.264312	3.913445
117	6	0	-7.765625	-3.266634	-0.084838
118	6	0	-6.106354	-4.033135	1.535895
119	8	0	-6.117311	-3.229985	3.810953
120	6	0	-7.721082	2.258435	2.304271
121	6	0	-6.003789	1.531847	3.882767
122	8	0	-6.043538	-0.717189	4.774294
123	6	0	-8.364601	-3.335871	-1.489683
124	6	0	-6.650446	-4.050417	0.253675
125	1	0	-5.292350	-4.699310	1.794626
126	6	0	-4.844271	-2.668900	3.994737
127	6	0	-8.282203	3.368721	1.421540
128	6	0	-6.567895	2.506668	3.063949
129	1	0	-5.162801	1.770057	4.520511
130	6	0	-4.806615	-1.290957	4.469107
131	1	0	-8.048633	-4.290852	-1.918250
132	6	0	-7.760261	-2.240498	-2.365506
133	8	0	-6.118871	-4.954554	-0.697298
134	6	0	-7.663358	3.287553	0.026868
135	1	0	-7.950605	4.315296	1.856640
136	8	0	-6.033069	3.814327	3.071521
137	6	0	-8.298307	-0.943563	-2.450534
138	6	0	-6.608668	-2.510554	-3.121390
139	6	0	-4.858961	-4.692593	-1.249993
140	6	0	-2.416094	-2.746074	3.987016
141	6	0	-8.190100	2.452300	-0.971412
142	6	0	-6.543815	4.065387	-0.315408
143	6	0	-4.770200	4.050646	2.518788
144	6	0	-2.388110	-1.327661	4.424281
145	6	0	-7.716109	0.071343	-3.228506
146	6	0	-6.011546	-1.540253	-3.924185
147	8	0	-6.100050	-3.828992	-3.148793
148	6	0	-4.848442	-4.088577	-2.576009
149	6	0	-7.677862	2.394380	-2.278713

150	6	0	-6.013962	4.052288	-1.603951
151	8	0	-5.993901	4.966220	0.629422
152	6	0	-4.747757	4.677164	1.201512
153	6	0	-8.287402	1.484521	-3.344138
154	6	0	-6.552236	-0.257429	-3.941296
155	1	0	-5.173901	-1.796911	-4.559597
156	6	0	-2.438892	-4.842591	-1.281989
157	6	0	-6.580959	3.221125	-2.569452
158	1	0	-5.196363	4.714391	-1.863692
159	6	0	-2.348427	4.165587	2.621946
160	1	0	-7.961432	1.875142	-4.311910
161	8	0	-5.985319	0.729632	-4.776718
162	6	0	-2.425173	-4.234954	-2.634942
163	8	0	-6.056878	3.270978	-3.888450
164	6	0	-2.324262	4.820608	1.290805
165	6	0	-4.751864	1.295382	-4.456920
166	6	0	-4.786936	2.698699	-4.056624
167	6	0	-2.337027	1.314179	-4.338388
168	6	0	-2.359799	2.761491	-3.994970
169	6	0	-3.682271	-3.877311	-3.251795
170	6	0	-3.703796	-5.068867	-0.625220
171	6	0	-3.701038	-3.382250	3.786411
172	6	0	-3.628108	-0.639223	4.682096
173	6	0	-3.575407	0.620890	-4.594286
174	6	0	-3.645110	3.417558	-3.869289
175	6	0	-3.619412	3.808065	3.208148
176	6	0	-3.576695	5.057021	0.607383
177	1	0	-3.674877	-3.500947	-4.268292
178	1	0	-3.727268	-5.581100	0.329805
179	1	0	-3.546901	-0.404572	-4.942231
180	1	0	-3.731891	-4.427007	3.499050
181	1	0	-3.674693	4.474735	-3.632008
182	1	0	-3.602112	0.362259	5.094147
183	1	0	-3.633885	3.411992	4.216886
184	1	0	-3.581622	5.588550	-0.337800
185	7	0	-1.194470	3.337504	-3.760643
186	7	0	-1.143612	0.755734	-4.379064
187	7	0	-1.122281	5.123048	0.819808
188	7	0	-1.178738	3.941016	3.198155
189	7	0	-1.189610	-0.783877	4.544140
190	7	0	-1.243778	-3.321970	3.771261
191	7	0	-1.250268	-5.116196	-0.759178
192	7	0	-1.236734	-4.044198	-3.190994
193	1	0	-9.203665	-0.719437	-1.893826
194	1	0	-9.144201	-1.808857	0.676550
195	1	0	-9.189217	0.765200	1.819910
196	1	0	-9.044968	1.829091	-0.723878
197	6	0	-9.825804	1.500968	-3.313350
198	1	0	-10.223256	0.872619	-4.116591
199	6	0	-9.820118	3.371679	1.378074
200	1	0	-10.238447	2.453747	0.952036
201	1	0	-10.175650	4.209262	0.770113
202	6	0	-9.881344	-1.426734	3.265148
203	1	0	-10.288370	-1.036889	2.326222
204	1	0	-10.261028	-0.798236	4.076781
205	6	0	-9.902403	-3.299970	-1.472834
206	1	0	-10.304792	-2.373380	-1.050106
207	1	0	-10.288601	-4.130202	-0.873599
208	52	0	0.290923	-4.703100	-2.013739
209	52	0	0.333988	-2.074526	4.176065
210	52	0	0.389708	2.054151	-4.034050
211	52	0	0.386636	4.621133	2.096430
212	1	0	-10.221750	3.480030	2.390416
213	1	0	-10.239159	1.132756	-2.368514
214	1	0	-10.270766	-2.440803	3.397667
215	1	0	-10.290209	-3.395133	-2.491884
216	1	0	-10.190526	2.522658	-3.456746
217	6	0	-5.671844	-0.189133	0.175814
218	6	0	-4.543594	0.262214	-0.764801
219	1	0	-6.614355	-0.330546	-0.366364
220	1	0	-5.419447	-1.138015	0.670963
221	1	0	-5.844730	0.565442	0.956043
222	6	0	-3.275992	0.619096	0.036407
223	1	0	-4.321958	-0.529946	-1.495986
224	1	0	-4.872754	1.143012	-1.339644
225	1	0	-3.507739	1.446918	0.722623
226	1	0	-2.968409	-0.236021	0.652839
227	6	0	-2.132166	1.022437	-0.885240
228	1	0	-2.395502	1.866605	-1.529016
229	1	0	-1.742109	0.187933	-1.475241
230	35	0	-0.562861	1.681465	0.205041
231	6	0	2.072328	-0.946406	-0.918610
232	1	0	2.298526	-1.730824	-1.647147
233	1	0	1.668663	-0.057794	-1.413023
234	6	0	3.253554	-0.636775	-0.007186
235	6	0	4.486438	-0.180757	-0.811489
236	1	0	3.516043	-1.531709	0.576038
237	1	0	2.967837	0.144274	0.709902
238	6	0	5.644363	0.186620	0.130282
239	1	0	4.803737	-0.991092	-1.487521
240	1	0	4.229019	0.680933	-1.446106
241	1	0	6.553844	0.433039	-0.429949
242	1	0	5.386288	1.054303	0.754705
243	1	0	5.879889	-0.653566	0.798788
244	35	0	0.539622	-1.686709	0.171471

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Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	8.313793	-3.406761	1.338381
2	6	0	7.721312	-2.307909	2.221223
3	6	0	7.709823	-3.325422	-0.060313
4	1	0	7.990683	-4.360088	1.765620
5	6	0	8.284291	-1.027050	2.351114
6	6	0	6.553390	-2.573610	2.956436
7	6	0	8.225341	-2.462685	-1.042305
8	6	0	6.588567	-4.096235	-0.409587
9	6	0	7.740606	-0.033523	3.188005

10	6	0	6.009121	-1.639483	3.832147
11	8	0	6.000417	-3.868987	2.885531
12	6	0	7.673538	-2.334934	-2.328047
13	6	0	6.007205	-3.999836	-1.671269
14	8	0	6.074655	-5.064927	0.489580
15	6	0	8.347038	1.364810	3.328957
16	6	0	6.600287	-0.380246	3.928143
17	1	0	5.170034	-1.900154	4.463863
18	6	0	4.759040	-4.111603	2.297320
19	6	0	8.278716	-1.401723	-3.379216
20	6	0	6.539179	-3.116079	-2.607872
21	1	0	5.172502	-4.638187	-1.935781
22	6	0	4.799936	-4.832287	1.028467
23	1	0	8.012548	1.750377	4.296140
24	6	0	7.788689	2.315626	2.267407
25	8	0	6.065429	0.550023	4.852181
26	6	0	7.744974	0.023474	-3.223615
27	1	0	7.925106	-1.759626	-4.350408
28	8	0	5.945754	-3.084776	-3.895040
29	6	0	8.366812	2.459114	0.994341
30	6	0	6.652120	3.095724	2.538192
31	6	0	4.810348	1.094696	4.552542
32	6	0	2.342534	-4.258161	2.308668
33	6	0	8.357345	1.010734	-2.428979
34	6	0	6.576631	0.389475	-3.910978
35	6	0	4.697232	-2.457884	-4.008989
36	6	0	2.375363	-5.050467	1.050917
37	6	0	7.857962	3.320062	0.004763
38	6	0	6.146075	4.001921	1.609694
39	8	0	6.059899	3.036101	3.822690
40	6	0	4.807328	2.431608	3.968426
41	6	0	7.835575	2.310935	-2.289051
42	6	0	6.047139	1.674558	-3.833748
43	8	0	5.979569	-0.552729	-4.777413
44	6	0	4.719914	-1.073090	-4.467490
45	6	0	8.462781	3.389401	-1.399418
46	6	0	6.740367	4.098784	0.352073
47	1	0	5.322093	4.654562	1.871778
48	6	0	2.384455	1.050586	4.503752
49	6	0	6.664849	2.608649	-3.005168
50	1	0	5.199426	1.957102	-4.443247
51	6	0	2.269081	-2.429199	-3.949375
52	1	0	8.165323	4.353804	-1.820833
53	8	0	6.245878	5.079589	-0.544083
54	6	0	2.383738	2.415235	3.910752
55	8	0	6.161649	3.925675	-2.958267
56	6	0	2.298509	-1.012776	-4.400599
57	6	0	4.967428	4.879223	-1.088901
58	6	0	4.920691	4.193328	-2.374470
59	6	0	2.546095	5.117231	-1.109319
60	6	0	2.505473	4.354697	-2.383121
61	6	0	3.644182	3.079525	3.668576
62	6	0	3.651816	0.434700	4.828928
63	6	0	3.577499	-3.821701	2.915880
64	6	0	3.665206	-5.303945	0.436926
65	6	0	3.836040	5.352007	-0.489678
66	6	0	3.738310	3.938041	-3.005552
67	6	0	3.527750	-3.119981	-3.766551
68	6	0	3.567746	-0.374795	-4.663163
69	1	0	3.649936	4.096265	3.293217
70	1	0	3.648474	-0.528551	5.325251
71	1	0	3.880809	5.925812	0.429128
72	1	0	3.553805	-3.347983	3.890467
73	1	0	3.706574	3.493136	-3.992851
74	1	0	3.706912	-5.895222	-0.470878
75	1	0	3.527976	-4.166602	-3.484174
76	1	0	3.570051	0.628543	-5.072004
77	7	0	1.300901	4.092155	-2.865742
78	7	0	1.377542	5.488666	-0.602665
79	7	0	1.131711	-0.413721	-4.534599
80	7	0	1.065806	-2.938211	-3.740866
81	7	0	1.209091	-5.446515	0.565185
82	7	0	1.140442	-4.011081	2.797676
83	7	0	1.210337	0.474196	4.677297
84	7	0	1.191741	2.912799	3.636610
85	1	0	9.240451	1.859356	0.754494
86	1	0	9.182953	-0.795373	1.786311
87	1	0	9.090939	-1.856175	-0.790832
88	1	0	9.268193	0.756586	-1.894209
89	6	0	9.998957	3.320596	-1.384754
90	1	0	10.387857	3.421898	-2.402768
91	1	0	10.381572	2.378893	-0.977246
92	6	0	9.816838	-1.452666	-3.379266
93	1	0	10.255558	-1.108843	-2.436646
94	1	0	10.212005	-0.818826	-4.179314
95	6	0	9.851748	-3.383317	1.320038
96	1	0	10.261220	-2.458776	0.899770
97	1	0	10.229739	-4.215048	0.717698
98	6	0	9.885595	1.333728	3.330310
99	1	0	10.306622	0.953920	2.393449
100	1	0	10.245459	0.690250	4.139123
101	52	0	-0.462465	-1.634312	-4.176474
102	52	0	-0.196061	4.891189	-1.766976
103	52	0	-0.367711	-4.840393	1.729432
104	52	0	-0.362862	1.690358	4.162921
105	1	0	10.157312	-2.479089	-3.546522
106	1	0	10.240334	-3.484818	2.338205
107	1	0	10.403972	4.133437	-0.774221
108	1	0	10.280264	2.342654	3.484969
109	6	0	-8.344594	3.338343	1.666613
110	6	0	-7.762534	2.159282	2.448615
111	6	0	-7.733744	3.380991	0.266217
112	1	0	-8.017777	4.247284	2.179422
113	6	0	-8.338247	0.877073	2.475798
114	6	0	-6.570630	2.341791	3.169725
115	6	0	-8.248943	2.606925	-0.788609
116	6	0	-6.613534	4.179580	-0.017366
117	6	0	-7.773060	-0.199906	3.185721
118	6	0	-6.003592	1.320651	3.926090
119	8	0	-6.011153	3.634663	3.212684
120	6	0	-7.702507	2.595816	-2.082292
121	6	0	-6.034057	4.193645	-1.284505

122	8	0	-6.088186	5.064869	0.959502
123	6	0	-8.371291	-1.608495	3.207005
124	6	0	-6.603140	0.062331	3.914523
125	1	0	-5.146502	1.513593	4.557192
126	6	0	-4.768589	3.917146	2.645322
127	6	0	-8.314570	1.769064	-3.215978
128	6	0	-6.567711	3.398131	-2.295100
129	1	0	-5.199382	4.852790	-1.492072
130	6	0	-4.810483	4.766163	1.459683
131	1	0	-8.035690	-2.073412	4.138365
132	6	0	-7.802364	-2.459983	2.068676
133	8	0	-6.069320	-0.955137	4.738950
134	6	0	-7.779622	0.336562	-3.197673
135	1	0	-7.965277	2.218799	-4.149698
136	8	0	-5.981576	3.483325	-3.583038
137	6	0	-8.371850	-2.474126	0.784109
138	6	0	-6.674977	-3.275601	2.268096
139	6	0	-4.817629	-1.484135	4.409810
140	6	0	-2.350482	4.007365	2.633328
141	6	0	-8.385017	-0.716493	-2.486484
142	6	0	-6.614166	0.034692	-3.918908
143	6	0	-4.734942	2.869326	-3.767449
144	6	0	-2.382564	4.932395	1.470208
145	6	0	-7.872859	-3.248514	-0.278976
146	6	0	-6.170453	-4.089021	1.256060
147	8	0	-6.084458	-3.360065	3.552467
148	6	0	-4.824479	-2.786254	3.752797
149	6	0	-7.857337	-2.020546	-2.460055
150	6	0	-6.073521	-1.248474	-3.946189
151	8	0	-6.025392	1.046877	-4.709643
152	6	0	-4.763363	1.536481	-4.358936
153	6	0	-8.483404	-3.179949	-1.679282
154	6	0	-6.763349	-4.066622	-0.005201
155	1	0	-5.349039	-4.766629	1.456718
156	6	0	-2.392324	-1.476733	4.395140
157	6	0	-6.683544	-2.250184	-3.196091
158	1	0	-5.226762	-1.474410	-4.579928
159	6	0	-2.305851	2.827469	-3.729708
160	1	0	-8.190663	-4.098760	-2.195120
161	8	0	-6.273737	-4.968451	-0.985006
162	6	0	-2.399416	-2.805711	3.726614
163	8	0	-6.182499	-3.567154	-3.259508
164	6	0	-2.342258	1.458139	-4.306337
165	6	0	-4.994024	-4.721284	-1.507524
166	6	0	-4.942996	-3.896279	-2.709683
167	6	0	-2.573186	-4.966612	-1.551531
168	6	0	-2.529560	-4.065819	-2.733344
169	6	0	-3.666852	-3.435725	3.432226
170	6	0	-3.653325	-0.858031	4.736035
171	6	0	-3.586656	3.539324	3.213239
172	6	0	-3.673816	5.276627	0.905375
173	6	0	-3.866472	-5.263571	-0.963737
174	6	0	-3.759500	-3.575672	-3.306477
175	6	0	-3.560909	3.502696	-3.474299
176	6	0	-3.614806	0.856031	-4.627283
177	1	0	-3.685303	-4.430245	3.001355
178	1	0	-3.639396	0.072903	5.290228
179	1	0	-3.915512	-5.932410	-0.111897
180	1	0	-3.558227	2.965054	4.131710
181	1	0	-3.724197	-3.021683	-4.236717
182	1	0	-3.713643	5.960449	0.064986
183	1	0	-3.554781	4.517430	-3.092829
184	1	0	-3.623623	-0.101681	-5.133722
185	7	0	-1.324950	-3.758333	-3.184620
186	7	0	-1.407181	-5.395436	-1.088340
187	7	0	-1.178624	0.865132	-4.490460
188	7	0	-1.099505	3.311546	-3.483212
189	7	0	-1.214072	5.353812	1.013045
190	7	0	-1.147967	3.684241	3.073215
191	7	0	-1.213179	-0.929725	4.624419
192	7	0	-1.207697	-3.300187	3.437174
193	1	0	-9.234947	-1.841402	0.597099
194	1	0	-9.258196	0.709665	1.922974
195	1	0	-9.113973	1.980006	-0.590280
196	1	0	-9.295558	-0.511780	-1.930386
197	6	0	-10.019250	-3.110103	-1.650549
198	1	0	-10.422879	-3.977000	-1.118494
199	6	0	-9.852501	1.820836	-3.203663
200	1	0	-10.287259	1.391324	-2.294968
201	1	0	-10.252312	1.264812	-4.057469
202	6	0	-9.882084	3.326597	1.636161
203	1	0	-10.293488	2.446023	1.131702
204	1	0	-10.251461	4.211116	1.108427
205	6	0	-9.909761	-1.591502	3.205681
206	1	0	-10.331916	-1.136100	2.303702
207	1	0	-10.277973	-1.023896	4.065980
208	52	0	0.350153	-2.126225	4.060626
209	52	0	0.365404	4.600190	2.084477
210	52	0	0.171870	-4.679379	-2.182513
211	52	0	0.420627	2.040153	-4.026302
212	1	0	-10.192257	2.858733	-3.272743
213	1	0	-10.398094	-2.211131	-1.153016
214	1	0	-10.277610	3.338738	2.656727
215	1	0	-10.295568	-2.613473	3.270803
216	1	0	-10.413137	-3.113085	-2.671663
217	6	0	-6.045677	0.083515	-0.055494
218	6	0	-4.682865	-0.390326	0.457649
219	1	0	-6.829175	-0.665679	0.081023
220	1	0	-6.348733	0.993596	0.475783
221	1	0	-5.988649	0.328315	-1.125090
222	6	0	-3.656015	0.728652	0.215130
223	1	0	-4.740223	-0.632398	1.530159
224	1	0	-4.373208	-1.308034	-0.063713
225	1	0	-3.685920	1.006710	-0.848057
226	1	0	-3.941234	1.623036	0.787685
227	6	0	-2.247623	0.298678	0.582024
228	1	0	-1.920933	-0.589757	0.041622
229	1	0	-2.091278	0.166412	1.657000
230	35	0	-0.951650	1.743929	0.019483
231	6	0	2.312924	-0.209429	0.841153
232	1	0	1.867568	0.783250	0.732245
233	1	0	2.368160	-0.489244	1.898307

234	6	0	3.639622	-0.378422	0.110984
235	6	0	4.792536	0.456260	0.687183
236	1	0	3.507181	-0.120186	-0.949577
237	1	0	3.937187	-1.437118	0.139799
238	6	0	6.032948	0.167605	-0.168339
239	1	0	4.548561	1.528596	0.672057
240	1	0	4.972898	0.176998	1.735972
241	1	0	6.942478	0.614752	0.237217
242	1	0	6.187703	-0.916964	-0.237316
243	1	0	5.882989	0.550135	-1.186231
244	53	0	0.898736	-1.600681	-0.067192

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Atom	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	8.312050	-3.539539	1.031460
2	6	0	7.720974	-2.520772	2.005865
3	6	0	7.703249	-3.329202	-0.351627
4	1	0	7.988000	-4.526279	1.373358
5	6	0	8.285207	-1.256068	2.245754
6	6	0	6.549887	-2.847468	2.710443
7	6	0	8.216890	-2.376143	-1.246864
8	6	0	6.578924	-4.061064	-0.766880
9	6	0	7.743701	-0.337219	3.165675
10	6	0	6.005310	-1.990226	3.660814
11	8	0	6.000003	-4.134911	2.535550
12	6	0	7.661549	-2.124691	-2.512189
13	6	0	5.992352	-3.842161	-2.010747
14	8	0	6.073526	-5.112549	0.039232
15	6	0	8.361246	1.039009	3.435466
16	6	0	6.602190	-0.747414	3.871644
17	1	0	5.163306	-2.302974	4.264457
18	6	0	4.758022	-4.343285	1.934114
19	6	0	8.272105	-1.102864	-3.474648
20	6	0	6.524600	-2.873923	-2.860324
21	1	0	5.153998	-4.449333	-2.331350
22	6	0	4.799942	-4.946316	0.605143
23	1	0	8.024804	1.336290	4.432869
24	6	0	7.818393	2.091995	2.465183
25	8	0	6.069402	0.091977	4.879934
26	6	0	7.749803	0.307457	-3.192955
27	1	0	7.916408	-1.369589	-4.473979
28	8	0	5.928952	-2.717762	-4.137322
29	6	0	8.416854	2.369624	1.223554
30	6	0	6.667933	2.830470	2.791674
31	6	0	4.813587	0.657115	4.625308
32	6	0	2.343932	-4.539996	1.953352
33	6	0	8.370420	1.216763	-2.315214
34	6	0	6.585402	0.742068	-3.845786
35	6	0	4.685498	-2.074968	-4.187667
36	6	0	2.380095	-5.213061	0.628068
37	6	0	7.907091	3.312256	0.310556
38	6	0	6.164036	3.816430	1.947086
39	8	0	6.063979	2.645291	4.057579
40	6	0	4.810199	2.033716	4.144304
41	6	0	7.862413	2.506166	-2.063346
42	6	0	6.068576	2.020553	-3.656919
43	8	0	5.977837	-0.116102	-4.789615
44	6	0	4.716305	-0.654271	-4.520410
45	6	0	8.505552	3.499190	-1.086066
46	6	0	6.774939	4.041516	0.714104
47	1	0	5.328187	4.431333	2.258157
48	6	0	2.389800	0.606242	4.552180
49	6	0	6.694941	2.874599	-2.751780
50	1	0	5.223856	2.363242	-4.239210
51	6	0	2.258534	-2.034102	-4.101231
52	1	0	8.214461	4.498861	-1.421106
53	8	0	6.285314	5.101439	-0.088991
54	6	0	2.388177	2.011981	4.065813
55	8	0	6.203996	4.188821	-2.598892
56	6	0	2.295881	-0.582759	-4.425540
57	6	0	5.006971	4.969077	-0.653365
58	6	0	4.961306	4.417277	-2.002321
59	6	0	2.589204	5.242653	-0.667028
60	6	0	2.548480	4.616418	-2.014264
61	6	0	3.646738	2.699157	3.886009
62	6	0	3.656566	-0.026493	4.842767
63	6	0	3.577070	-4.137195	2.587802
64	6	0	3.668361	-5.386821	-0.015672
65	6	0	3.877385	5.395556	-0.017454
66	6	0	3.781766	4.247142	-2.666177
67	6	0	3.513231	-2.747480	-3.994451
68	6	0	3.568233	0.066549	-4.643652
69	1	0	3.650450	3.741768	3.590138
70	1	0	3.653676	-1.025274	5.262905
71	1	0	3.921331	5.874522	0.954155
72	1	0	3.555741	-3.755266	3.602117
73	1	0	3.752806	3.903761	-3.693274
74	1	0	3.711870	-5.894256	-0.972744
75	1	0	3.507495	-3.814604	-3.803874
76	1	0	3.575786	1.102726	-4.960175
77	7	0	1.345288	4.420986	-2.532102
78	7	0	1.422341	5.576833	-0.131594
79	7	0	1.133706	0.034578	-4.493835
80	7	0	1.054305	-2.551239	-3.925523
81	7	0	1.216443	-5.577336	0.111099
82	7	0	1.140579	-4.352691	2.467914
83	7	0	1.217749	0.011250	4.669496
84	7	0	1.194747	2.523815	3.824596
85	1	0	9.299526	1.804008	0.939191
86	1	0	9.184363	-0.978138	1.702988
87	1	0	9.086093	-1.800076	-0.942238
88	1	0	9.277895	0.907286	-1.804155
89	6	0	10.040786	3.414860	-1.089142
90	1	0	10.423836	3.600934	-2.097272
91	1	0	10.416320	2.437419	-0.768560
92	6	0	9.809939	-1.164320	-3.480967
93	1	0	10.251383	-0.909617	-2.511757

94	1	0	10.208981	-0.463768	-4.221164
95	6	0	9.849725	-3.516838	1.012356
96	1	0	10.260380	-2.559560	0.674786
97	1	0	10.225380	-4.292820	0.338459
98	6	0	9.899375	0.991863	3.441956
99	1	0	10.321871	0.693062	2.476896
100	1	0	10.247795	0.274374	4.191219
101	1	0	10.143194	-2.173838	-3.740202
102	1	0	10.239694	-3.708440	2.016906
103	1	0	10.458189	4.167249	-0.413010
104	1	0	10.303348	1.978512	3.688798
105	52	0	-0.469647	-1.199935	-4.225058
106	52	0	-0.148130	5.119974	-1.360051
107	52	0	-0.359881	-5.087167	1.322945
108	52	0	-0.358353	1.254179	4.238906
109	6	0	-8.335896	3.171729	1.978631
110	6	0	-7.761384	1.918513	2.642113
111	6	0	-7.718074	3.351278	0.590402
112	1	0	-8.007962	4.024282	2.580041
113	6	0	-8.348570	0.643150	2.558862
114	6	0	-6.559149	2.026328	3.360514
115	6	0	-8.227419	2.678006	-0.533659
116	6	0	-6.604327	4.182669	0.381792
117	6	0	-7.778129	-0.498510	3.155320
118	6	0	-5.986746	0.936098	4.008129
119	8	0	-5.995627	3.308247	3.515239
120	6	0	-7.687852	2.798935	-1.825655
121	6	0	-6.026373	4.318744	-0.878348
122	8	0	-6.077965	4.974311	1.436141
123	6	0	-8.379485	-1.903601	3.058527
124	6	0	-6.594671	-0.311706	3.885597
125	1	0	-5.120354	1.063530	4.642729
126	6	0	-4.754362	3.644216	2.977568
127	6	0	-8.309408	2.078599	-3.025418
128	6	0	-6.556987	3.623427	-1.962178
129	1	0	-5.191734	4.994965	-1.023051
130	6	0	-4.798227	4.624680	1.897325
131	1	0	-8.043071	-2.446206	3.946629
132	6	0	-7.814119	-2.657427	1.850988
133	8	0	-6.063691	-1.404975	4.606002
134	6	0	-7.784995	0.645773	-3.128748
135	1	0	-7.958133	2.604172	-3.917870
136	8	0	-5.963499	3.841337	-3.232903
137	6	0	-8.381794	-2.547925	0.570126
138	6	0	-6.692303	-3.496510	1.972882
139	6	0	-4.815136	-1.910509	4.234736
140	6	0	-2.337287	3.724887	2.959620
141	6	0	-8.404015	-0.468537	-2.530606
142	6	0	-6.603619	0.413077	-3.849010
143	6	0	-4.715498	3.246999	-3.470613
144	6	0	-2.369319	4.781071	1.911275
145	6	0	-7.886343	-3.216857	-0.564062
146	6	0	-6.193570	-4.212256	0.887152
147	8	0	-6.095740	-3.708041	3.240798
148	6	0	-4.830391	-3.161449	3.485598
149	6	0	-7.870877	-1.768746	-2.611378
150	6	0	-6.061539	-0.861454	-3.988954
151	8	0	-6.009502	1.498341	-4.527708
152	6	0	-4.745870	1.954372	-4.145479
153	6	0	-8.498399	-3.001247	-1.950440
154	6	0	-6.782394	-4.065448	-0.367835
155	1	0	-5.375196	-4.909873	1.022158
156	6	0	-2.390653	-1.920987	4.228245
157	6	0	-6.684981	-1.927377	-3.346422
158	1	0	-5.206538	-1.027667	-4.629215
159	6	0	-2.283654	3.218296	-3.470182
160	1	0	-8.208917	-3.863442	-2.557916
161	8	0	-6.287508	-4.873599	-1.424629
162	6	0	-2.404225	-3.199503	3.467172
163	8	0	-6.188431	-3.234007	-3.523350
164	6	0	-2.325186	1.883570	-4.121551
165	6	0	-5.005216	-4.573396	-1.912196
166	6	0	-4.950131	-3.615908	-3.011028
167	6	0	-2.584537	-4.815284	-1.980058
168	6	0	-2.538522	-3.775743	-3.041706
169	6	0	-3.676354	-3.795932	3.122925
170	6	0	-3.647588	-1.317790	4.607227
171	6	0	-3.571969	3.198987	3.490906
172	6	0	-3.663897	5.193057	1.399071
173	6	0	-3.879478	-5.176203	-1.431622
174	6	0	-3.765211	-3.222919	-3.559082
175	6	0	-3.539818	3.867107	-3.152894
176	6	0	-3.597899	1.294275	-4.462615
177	1	0	-3.701730	-4.756563	2.621237
178	1	0	-3.627834	-0.430675	5.228807
179	1	0	-3.931552	-5.937857	-0.661862
180	1	0	-3.539034	2.523473	4.337256
181	1	0	-3.724465	-2.566392	-4.419385
182	1	0	-3.706544	5.965936	0.639976
183	1	0	-3.535274	4.855619	-2.707343
184	1	0	-3.606354	0.371523	-5.030069
185	7	0	-1.334590	-3.417653	-3.454940
186	7	0	-1.419306	-5.306409	-1.580175
187	7	0	-1.162733	1.306502	-4.360126
188	7	0	-1.073088	3.693723	-3.217568
189	7	0	-1.201354	5.245354	1.499368
190	7	0	-1.136810	3.345024	3.351661
191	7	0	-1.209226	-1.401180	4.504208
192	7	0	-1.213751	-3.682424	3.149926
193	1	0	-9.239451	-1.893049	0.444013
194	1	0	-9.277287	0.532474	2.006554
195	1	0	-9.083093	2.022667	-0.394938
196	1	0	-9.327112	-0.316809	-1.978270
197	6	0	-10.034025	-2.931526	-1.912671
198	1	0	-10.439104	-3.849797	-1.476747
199	6	0	-9.846600	2.142195	-3.003676
200	1	0	-10.282428	1.639378	-2.133976
201	1	0	-10.253647	1.665823	-3.901153
202	6	0	-9.873254	3.170116	1.940817
203	1	0	-10.285750	2.348212	1.346335
204	1	0	-10.236393	4.105886	1.505279
205	6	0	-9.917887	-1.883209	3.061616

206	1	0	-10.340262	-1.354110	2.200933
207	1	0	-10.283084	-1.387536	3.966488
208	52	0	0.346577	-2.566949	3.867376
209	52	0	0.381791	4.359648	2.471788
210	52	0	0.158257	-4.467130	-2.587132
211	52	0	0.437277	2.455751	-3.860152
212	1	0	-10.177419	3.184932	-2.981170
213	1	0	-10.410393	-2.090931	-1.320345
214	1	0	-10.273225	3.079170	2.955637
215	1	0	-10.306086	-2.906113	3.043121
216	1	0	-10.428762	-2.823442	-2.927769
217	6	0	-6.115089	0.043920	-0.009620
218	6	0	-4.755013	-0.614406	0.242238
219	1	0	-6.942508	-0.666299	0.037848
220	1	0	-6.298232	0.829489	0.733332
221	1	0	-6.127277	0.516136	-1.000270
222	6	0	-3.688165	0.490225	0.189253
223	1	0	-4.740413	-1.118856	1.220346
224	1	0	-4.552628	-1.381079	-0.521125
225	1	0	-3.825546	1.058076	-0.742539
226	1	0	-3.860772	1.196577	1.014821
227	6	0	-2.262404	-0.038639	0.247036
228	1	0	-2.031608	-0.730851	-0.565833
229	1	0	-1.994900	-0.489481	1.207170
230	53	0	-0.900335	1.641491	-0.030679
231	6	0	2.385526	-0.461518	0.906968
232	1	0	1.926707	0.531757	0.897669
233	1	0	2.446938	-0.841729	1.931813
234	6	0	3.713593	-0.525556	0.164538
235	6	0	4.781085	0.423011	0.721792
236	1	0	3.550049	-0.278963	-0.893958
237	1	0	4.100820	-1.555511	0.190278
238	6	0	6.047037	0.255289	-0.124451
239	1	0	4.425823	1.463580	0.682039
240	1	0	4.989678	0.192030	1.777056
241	1	0	6.833797	0.948273	0.170270
242	1	0	6.446630	-0.762374	-0.027804
243	1	0	5.818390	0.430105	-1.184863
244	53	0	0.993509	-1.765815	-0.141750

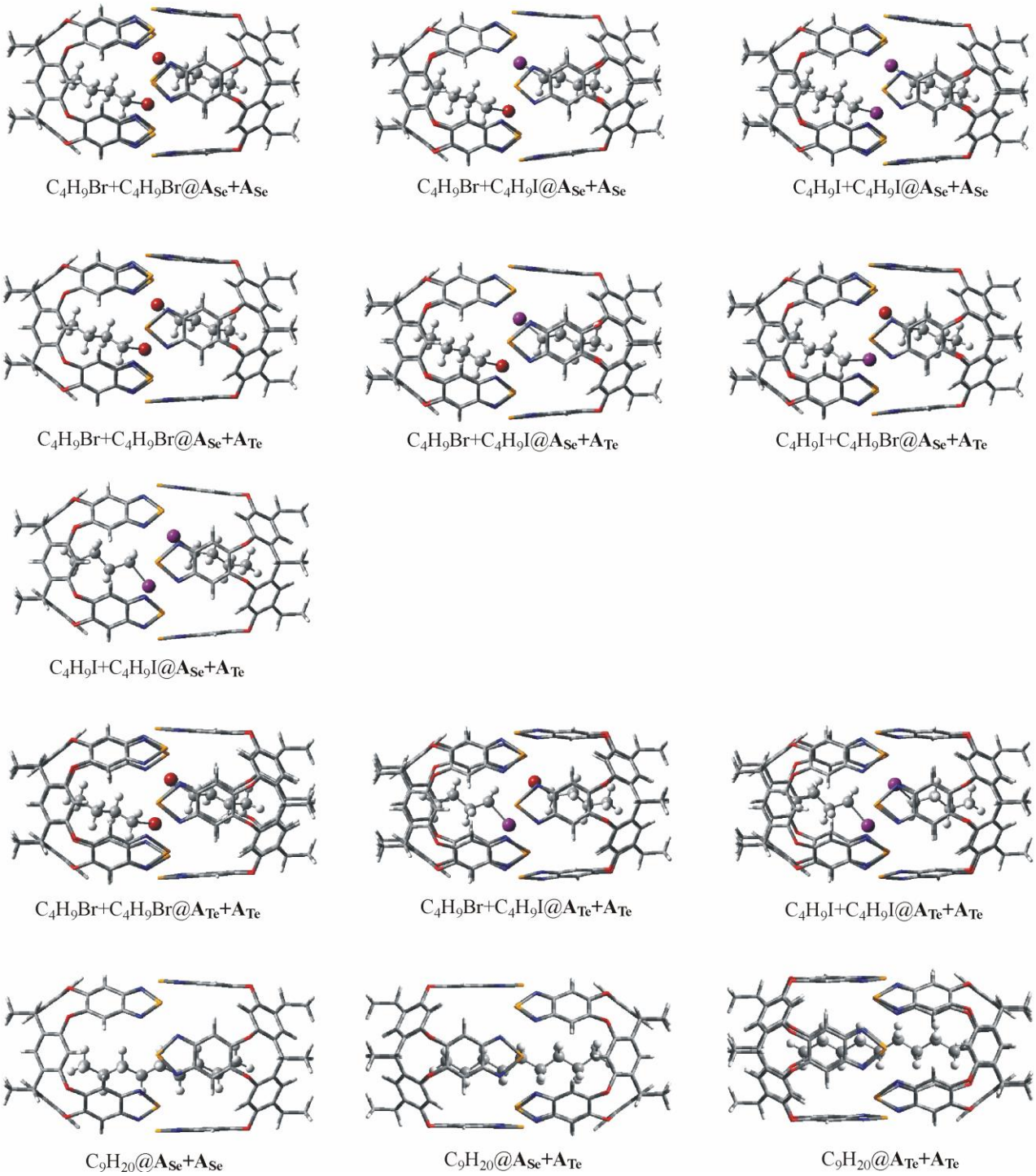


Figure 1S. Calculated encapsulated complexes **C_4H_9X+ C_4H_9X'@A'_{Y}+$A'_{Y'}$**, where X, X′ = Br, I and Y, Y′ = Se, Te.

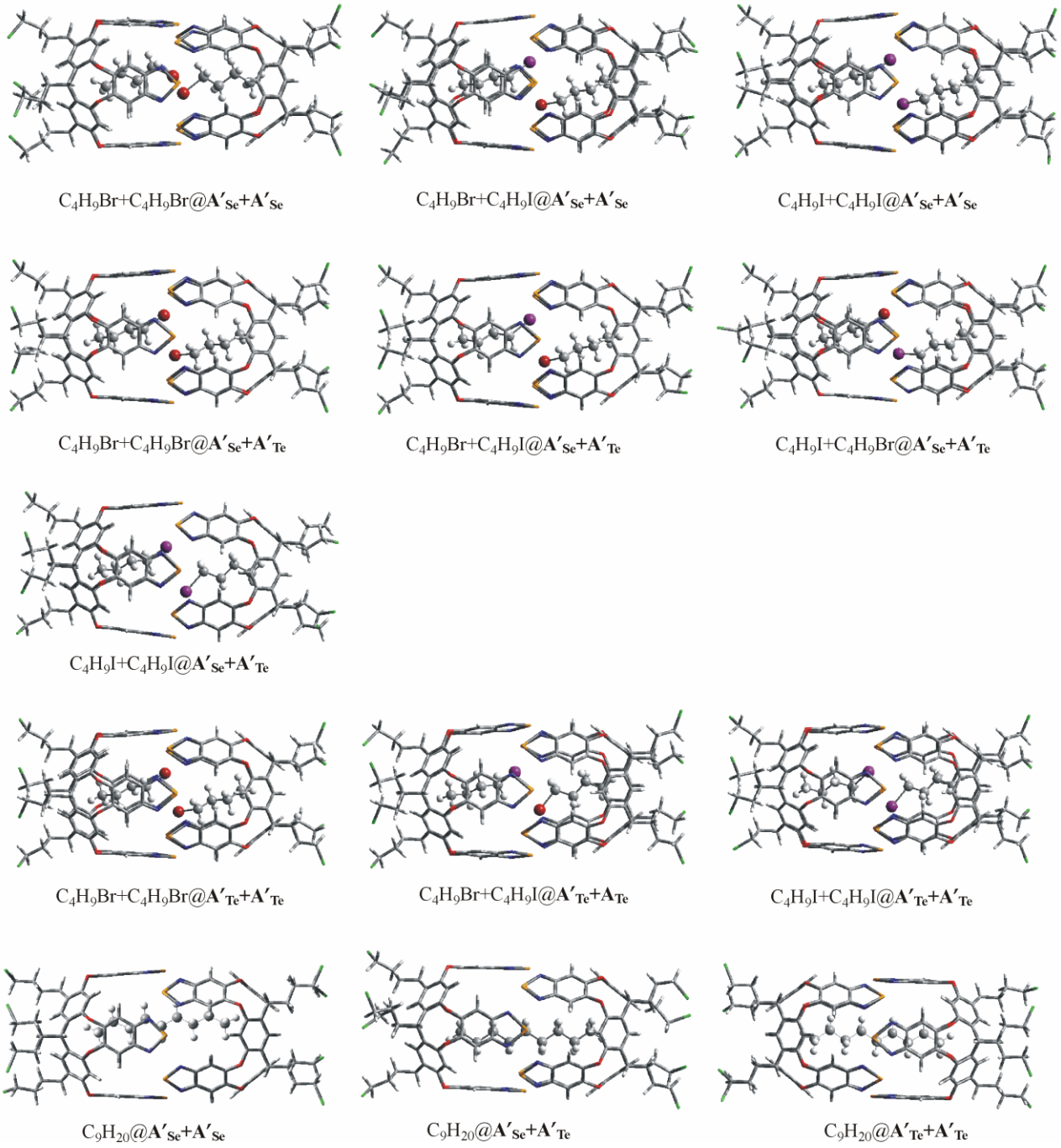


Figure 2S. Calculated encapsulated complexes **C_4H_9X+ C_4H_9X'@A'_Y+$A'_{Y'}$**, where X, X′ = Br, I and Y, Y′ = Se, Te.

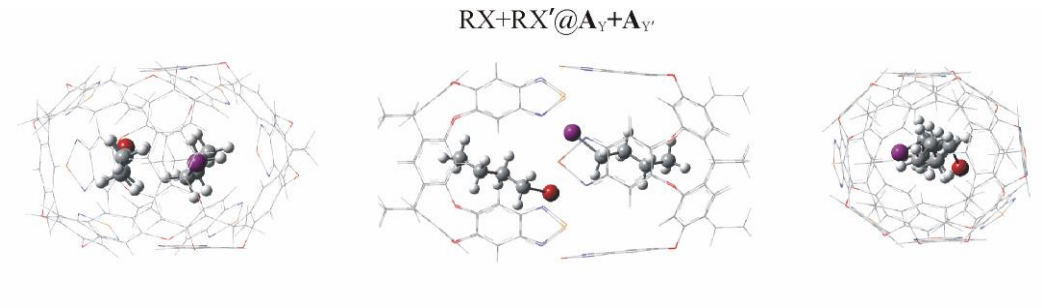


Figure 3S. Encapsulated complexes **RX+RX'@A$_Y$+A$_{Y'}$**, where X, X' = Br, I and Y, Y' = Se, Te from three points of view.

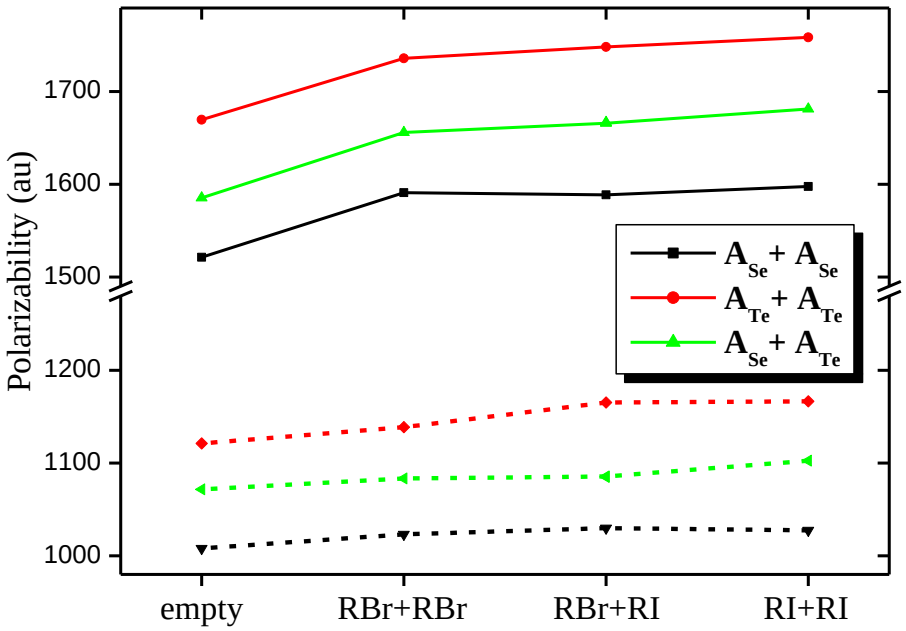


Figure 4S. Isotropic (Solid lines) and Anisotropic (Dot lines) polarizabilities of the encapsulated C_4H_9X+ C_4H_9X'@**A$_Y$+A$_{Y'}$** complexes with respect to the encapsulated contents at M06-2X/6-31G(d,p).

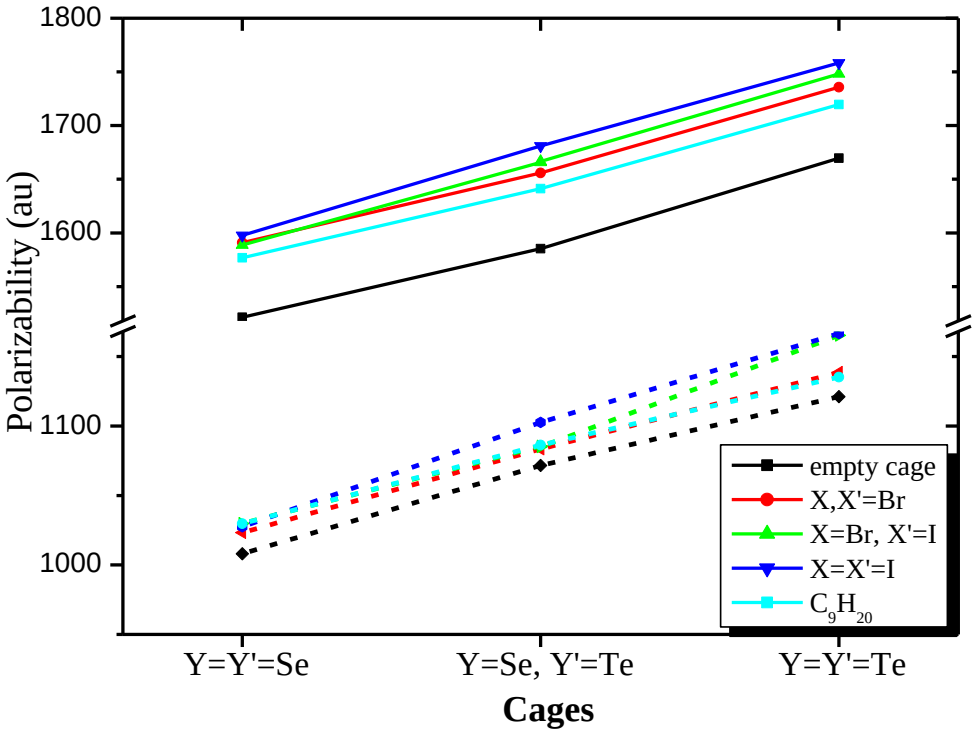


Figure 5S. Isotropic (Solid lines) and Anisotropic (Dot lines) polarizabilities of the encapsulated RX+RX'@$\mathbf{A_Y+A_{Y'}}$ complexes with respect to the cages at M06-2X/6-31G(d,p).

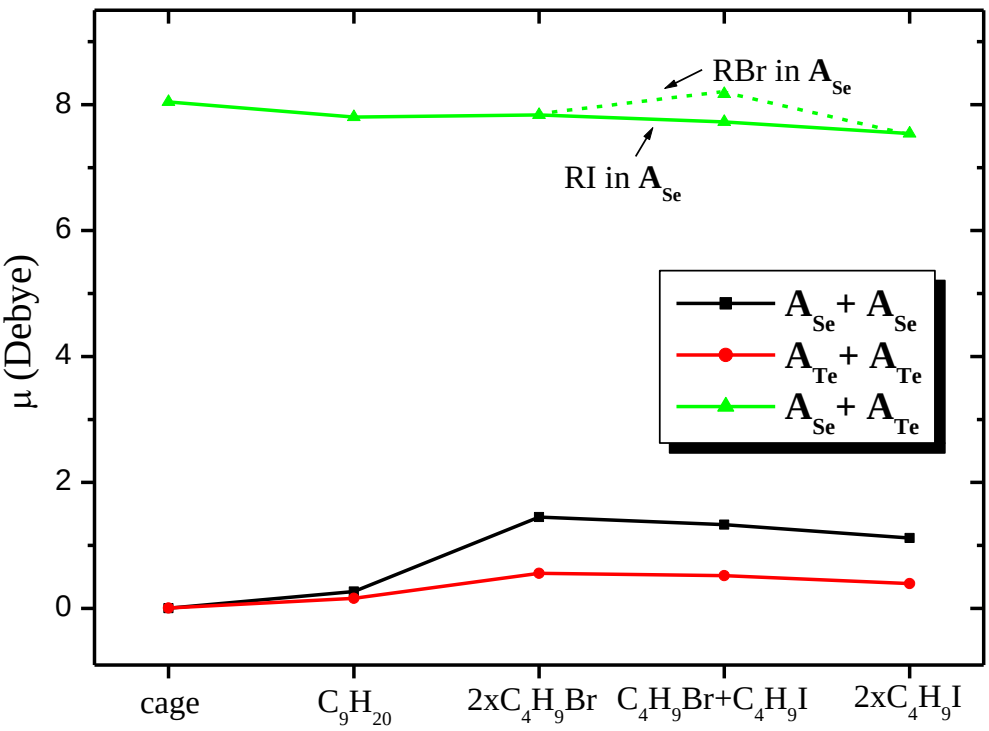


Figure 6S. Dipole moments μ of the encapsulated C_9H_{20}, $C_4H_9X+C_4H_9X'$@$\mathbf{A_Y+A_{Y'}}$ complexes at M06-2X/6-31G(d,p).

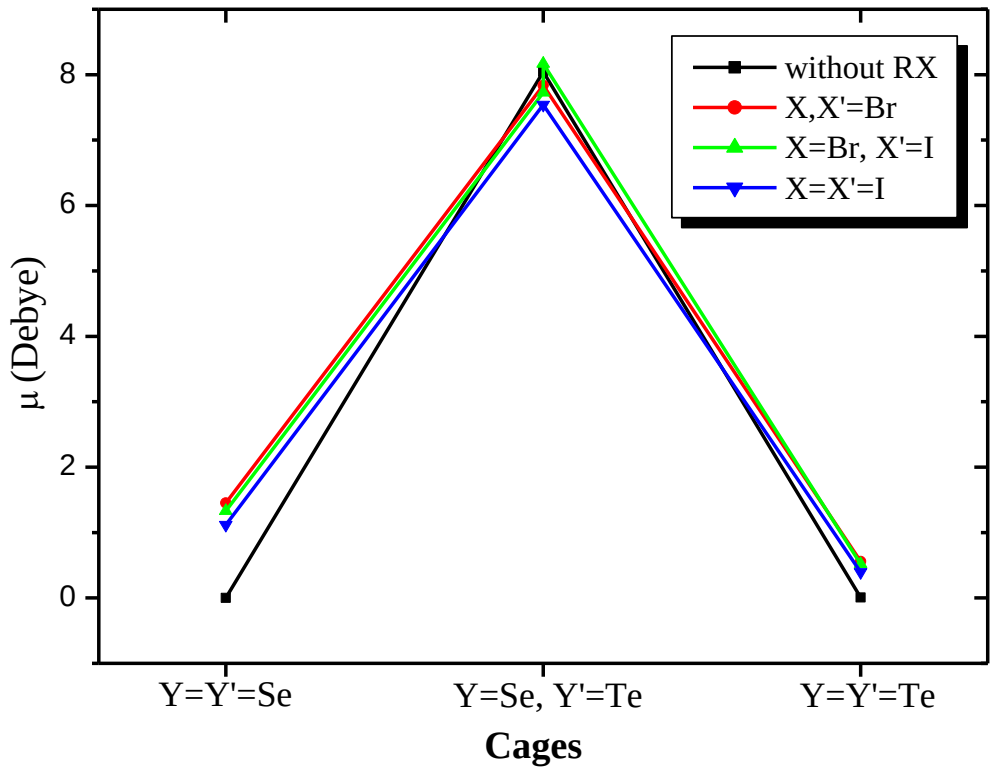


Figure 7S. Dipole moments μ of the encapsulated C_4H_9X+ C_4H_9X'@$\mathbf{A_Y}$+$\mathbf{A_{Y'}}$ complexes with respect to the cages at M06-2X/6-31G(d,p).

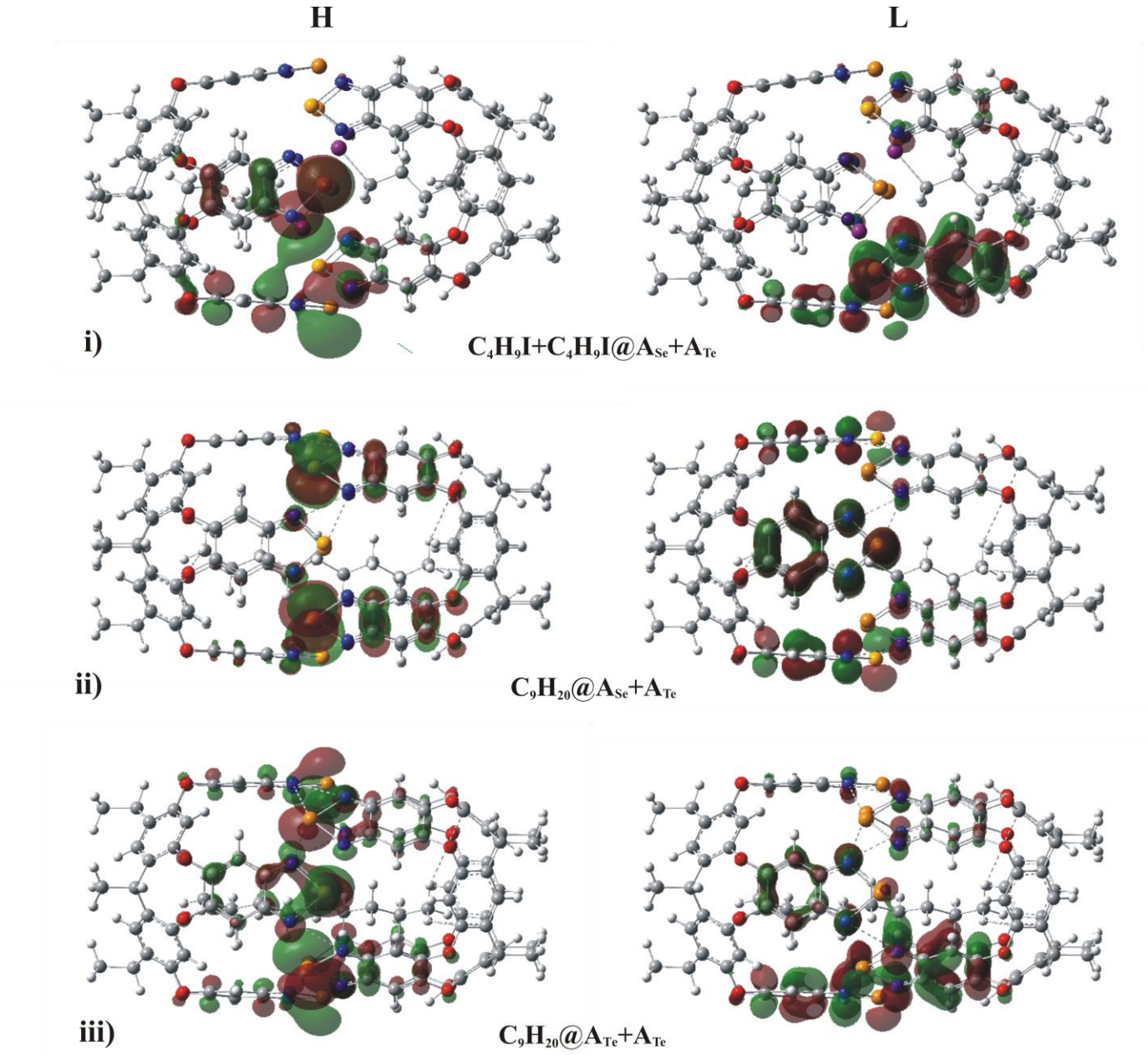


Fig. 8S. Molecular HOMO and LUMO MO of C_4H_9I+ C_4H_9I@$\mathbf{A_{Se}+A_{Te}}$, *n*-C_9H_{20} @$\mathbf{A_{Se}+A_{Te}}$, and *n*-C_9H_{20} @$\mathbf{A_{Te}+A_{Te}}$ complexes at M06-2X/6-31G(d.p)$_{C,H,O,N,Se,Br}$/LANL2TZ$_{I,Te}$

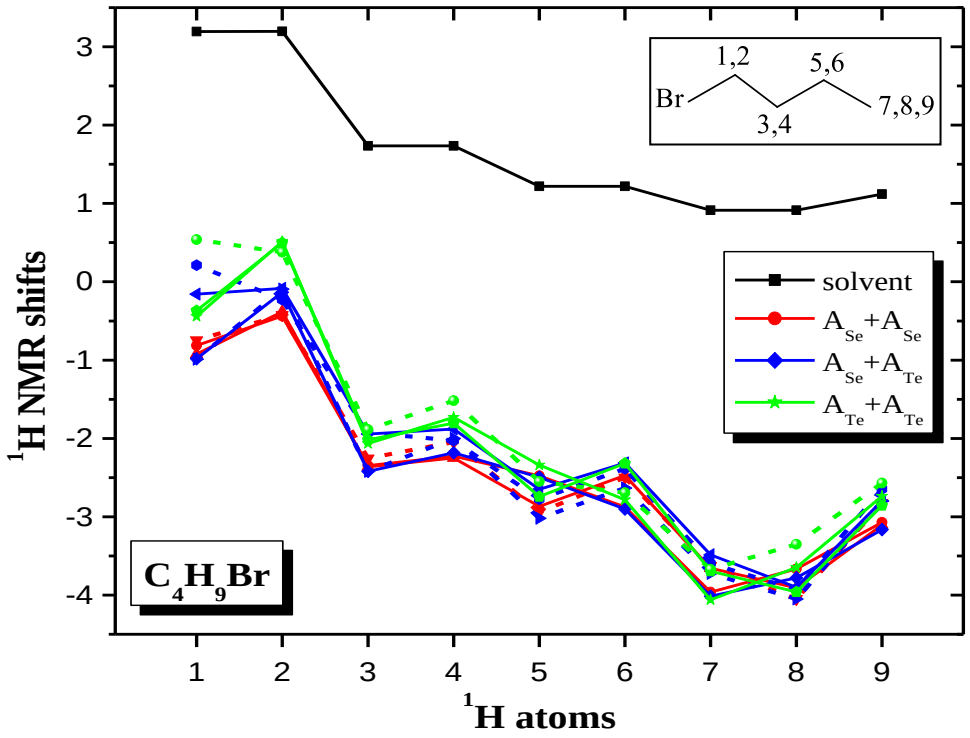


Figure 9S. ^{1}H NMR shifts (ppm) of the *1*-C_4H_9Br compound encapsulated and in solvent at M06-2X/6-31G(d,p) level of theory; A(R=CH_3).

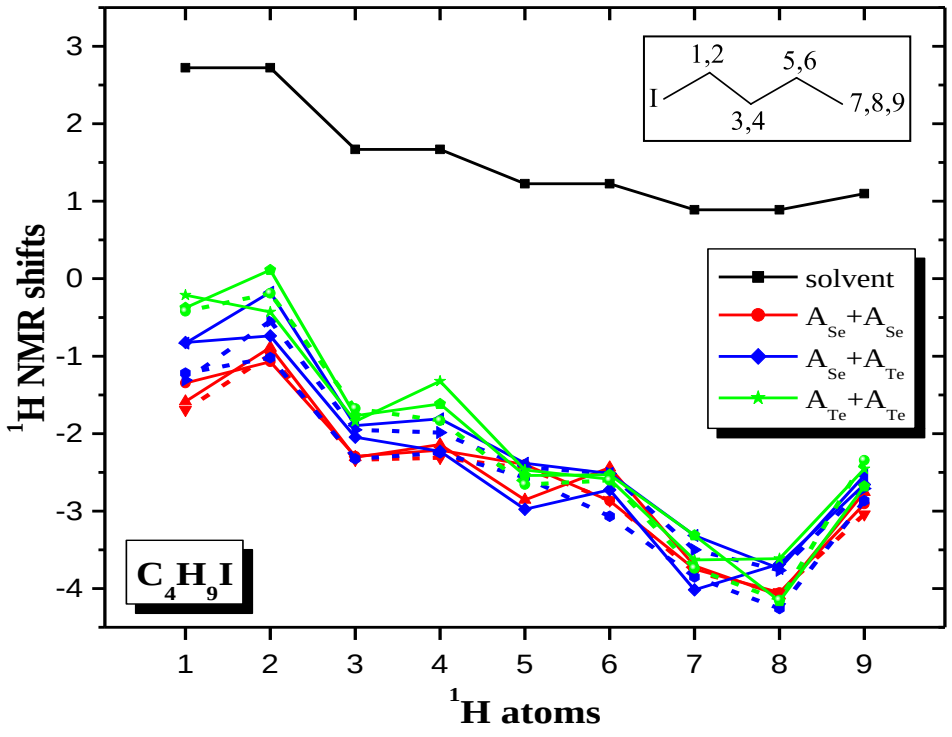


Figure 10S. ^{1}H NMR shifts (ppm) of the *1*-C_4H_9I compound encapsulated and in solvent at M06-2X/6-31G(d,p) level of theory; A(R=CH_3).

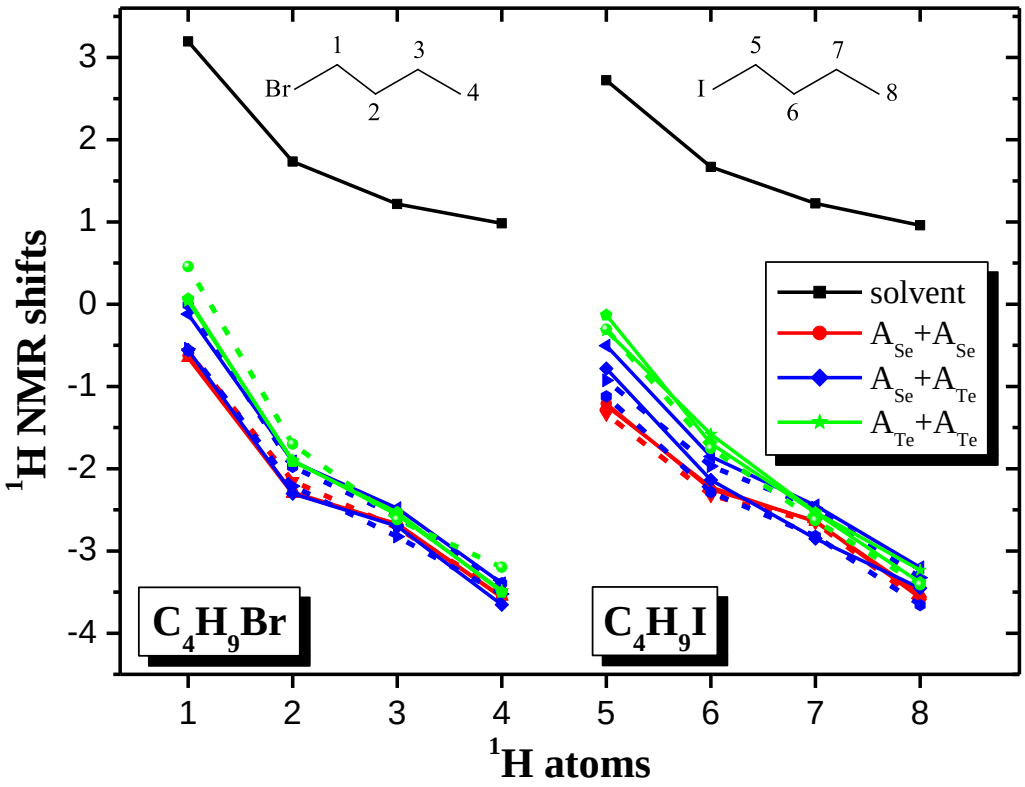


Figure 11S. ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br and 1-C_4H_9I compounds encapsulated and in solvent at M06-2X/6-31G(d,p) level of theory. Average ^{1}H NMR for the same C; A(R=CH_3).

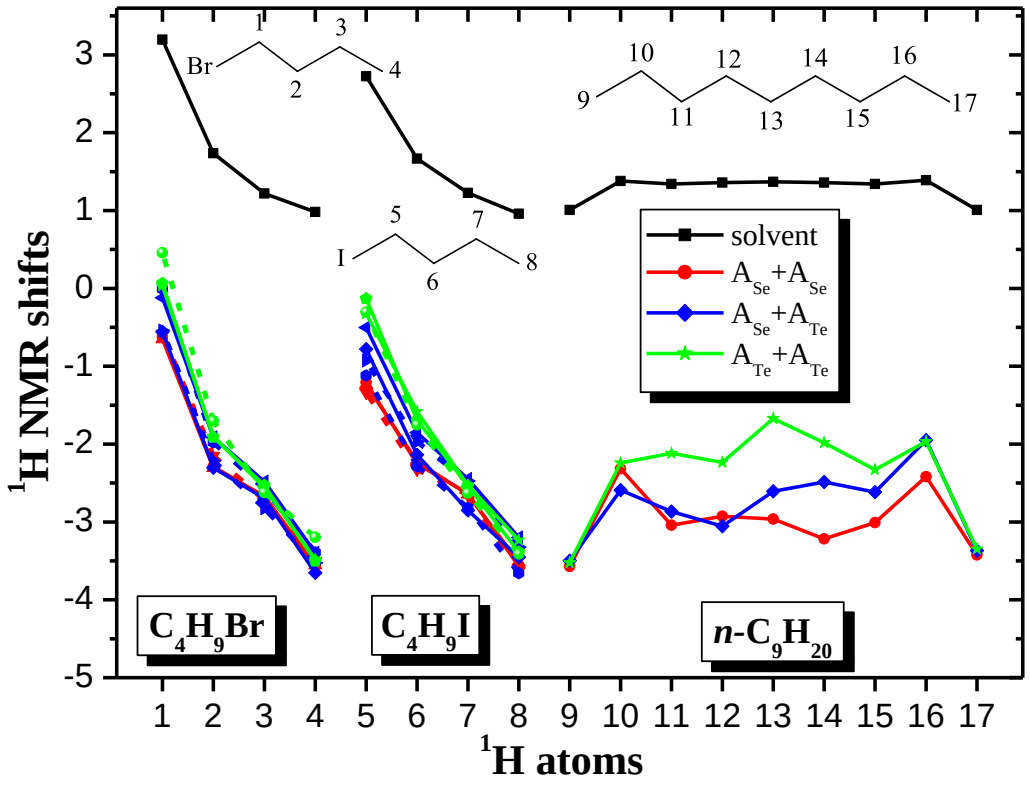


Figure 12S. ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and n-C_9H_{20} compounds encapsulated and in solvent at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C; A(R=CH_3).

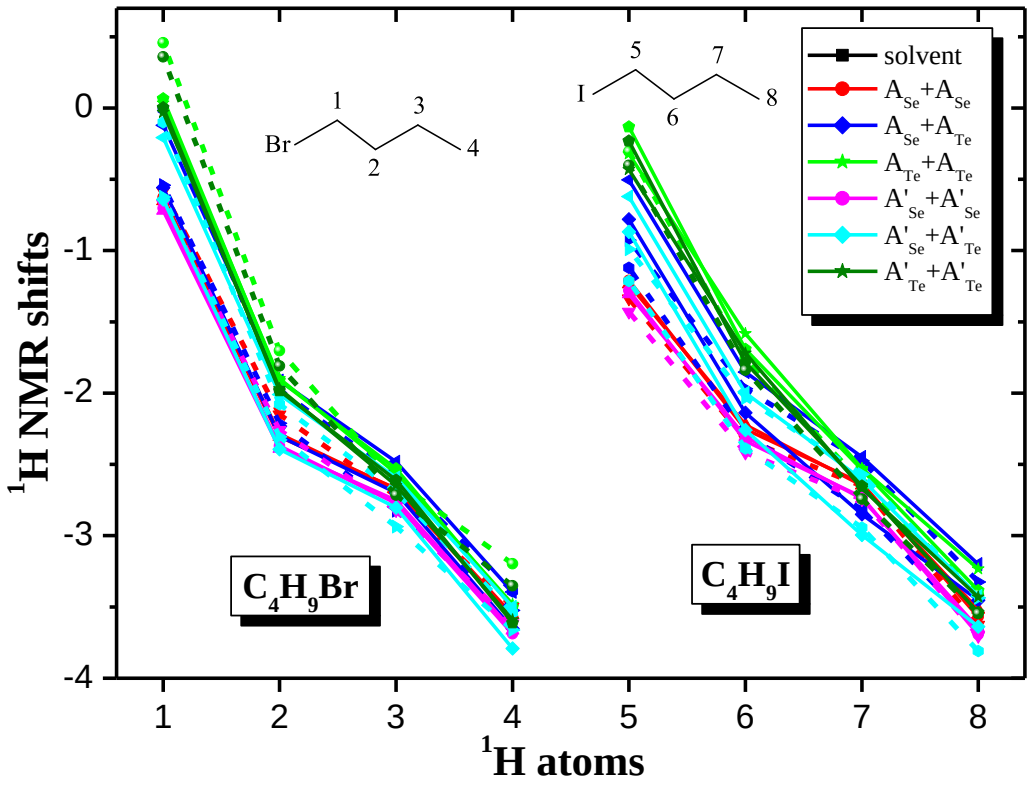


Figure 13S. ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br and 1-C_4H_9I encapsulated compounds at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C; A(R=CH_3); A′(R=$CH_2CH_2CH_2Cl$).

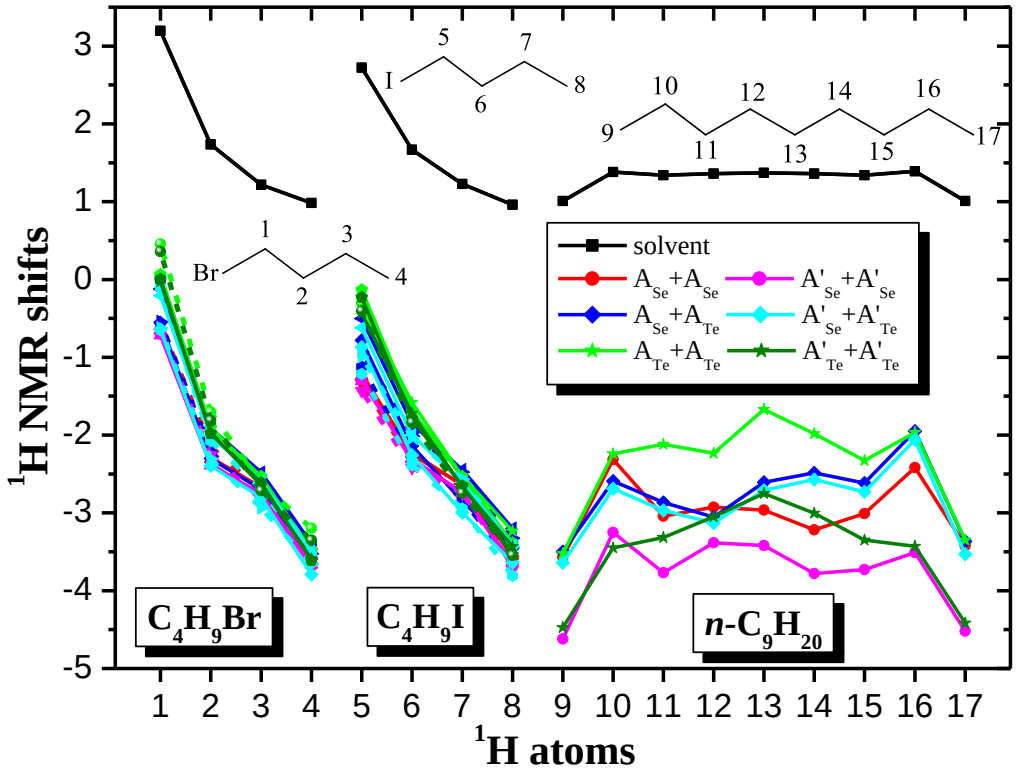


Figure 14S. ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and *n*-C_9H_{20} compounds encapsulated and in solvent at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C; A(R=CH_3); A′(R=$CH_2CH_2CH_2Cl$).

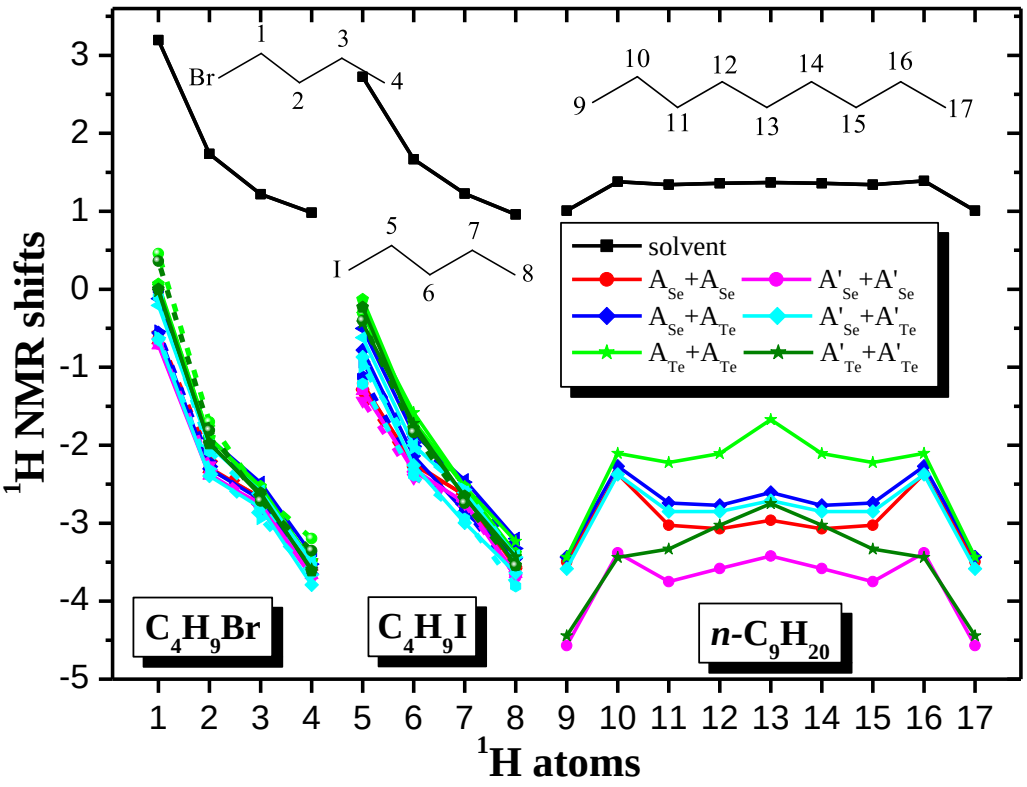


Figure 15S. ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and n-C_9H_{20} compounds encapsulated and in solvent at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C and for the symmetric C atoms; A(R=CH_3); A′(R=$CH_2CH_2CH_2Cl$).

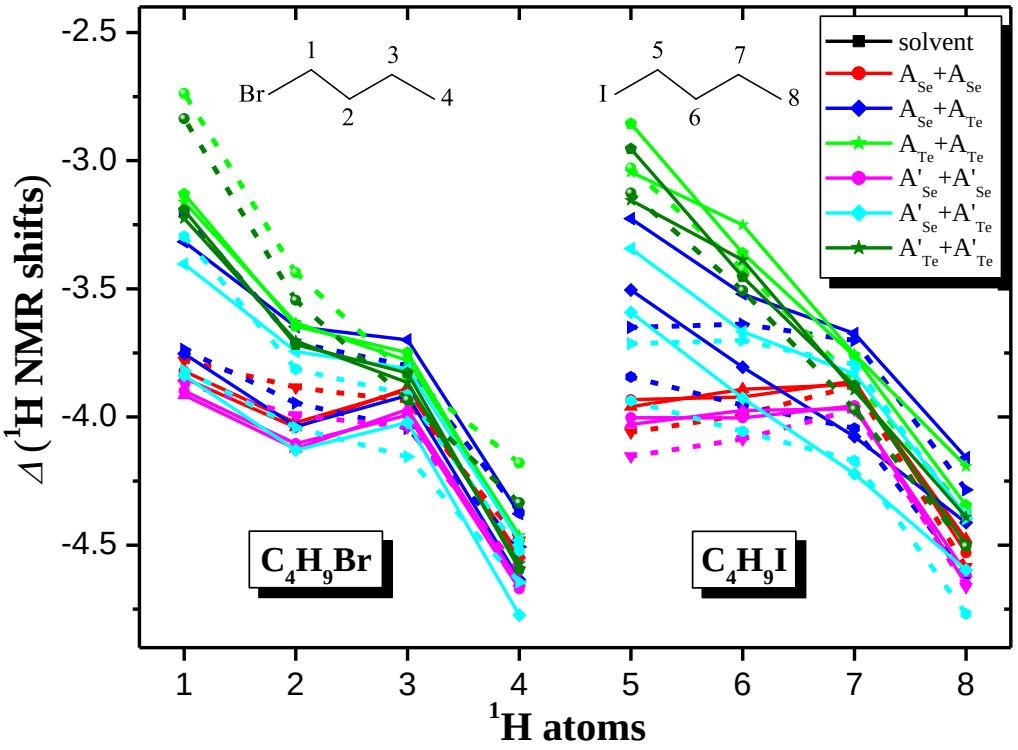


Figure 16S. Relative shifts of ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br and 1-C_4H_9I encapsulated compounds with respect to the free ones at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C; A(R=CH_3); A′(R=$CH_2CH_2CH_2Cl$).

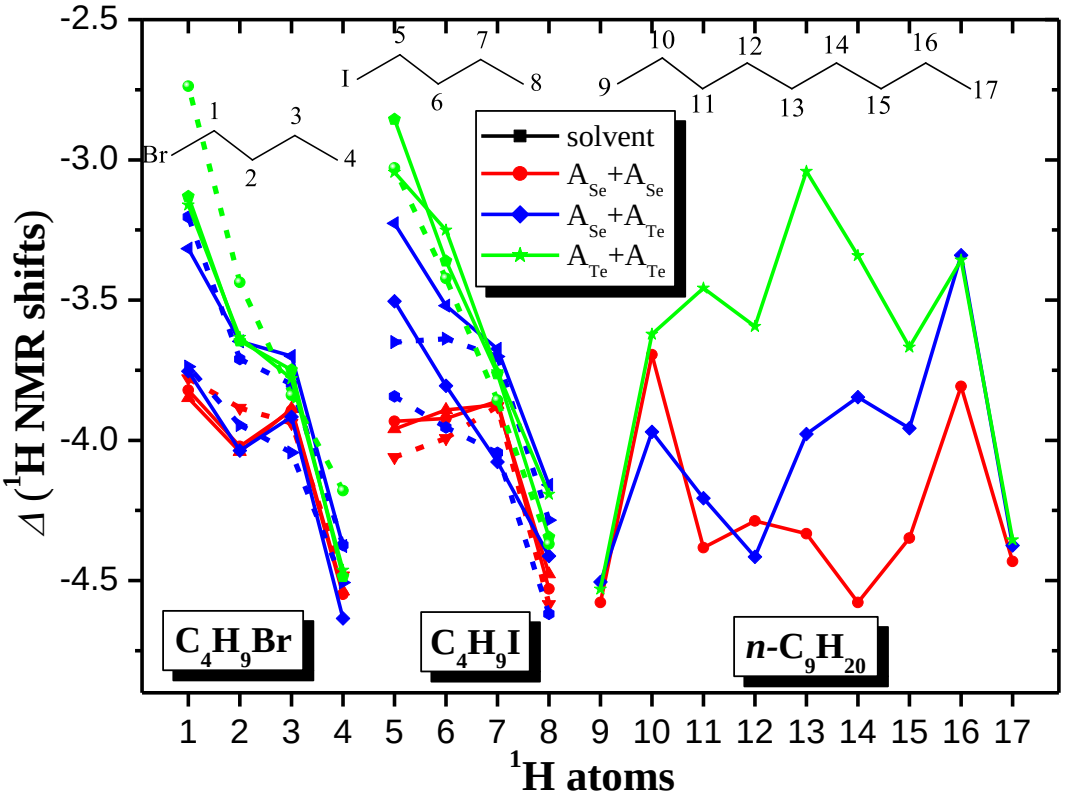


Figure 17S. Relative shifts of ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and *n*-C_9H_{20} encapsulated compounds with respect to the free ones at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C; A(R=CH_3).

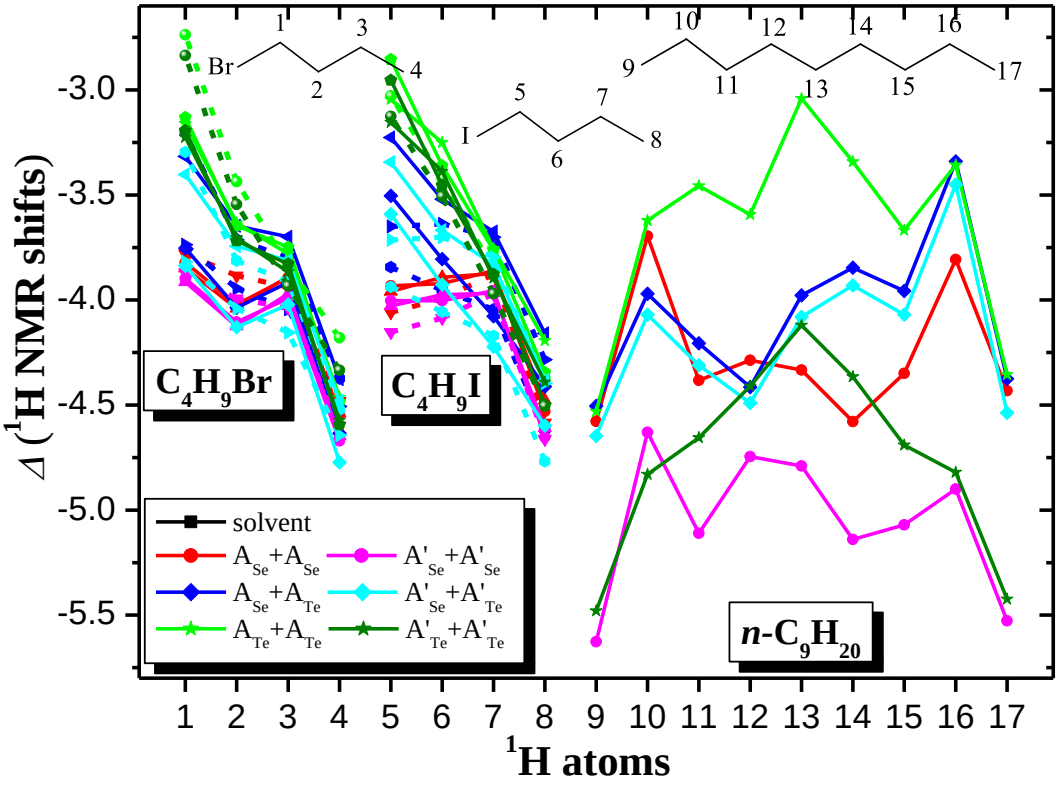


Figure 18S. Relative shifts of ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and *n*-C_9H_{20} encapsulated compounds with respect to the free ones at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C; A(R=CH_3); A′(R=$CH_2CH_2CH_2Cl$).

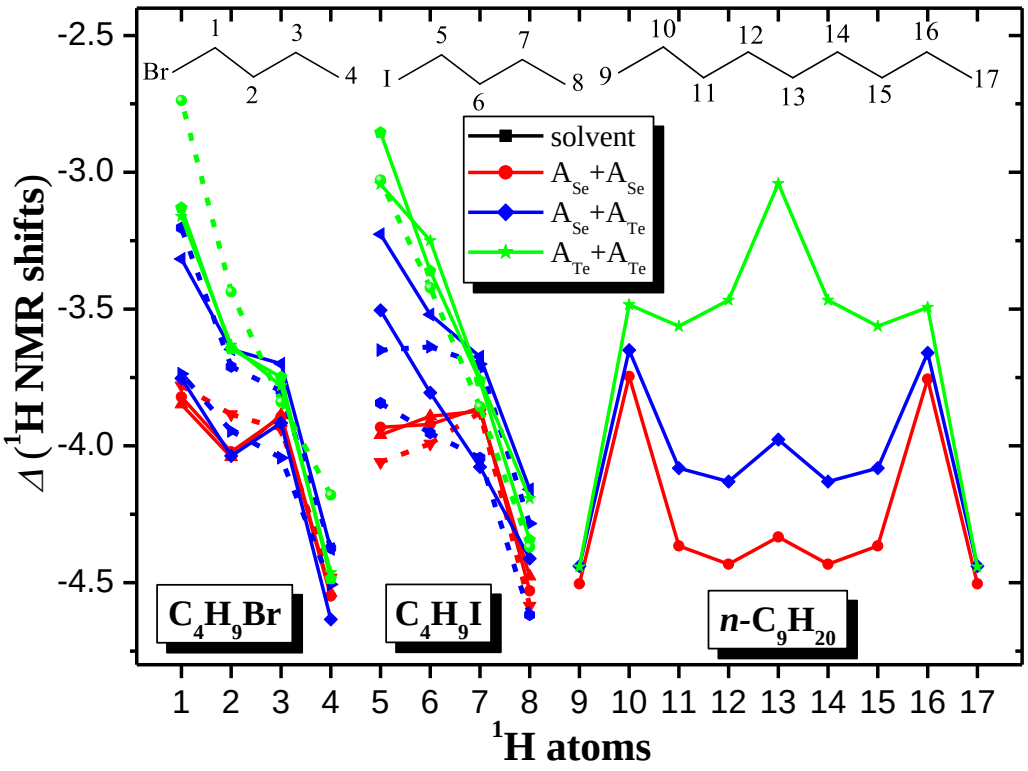


Figure 19S. Relative shifts of ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and *n*-C_9H_{20} encapsulated compounds with respect to the free compounds at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C and for the symmetric C atoms; A(R=CH_3).

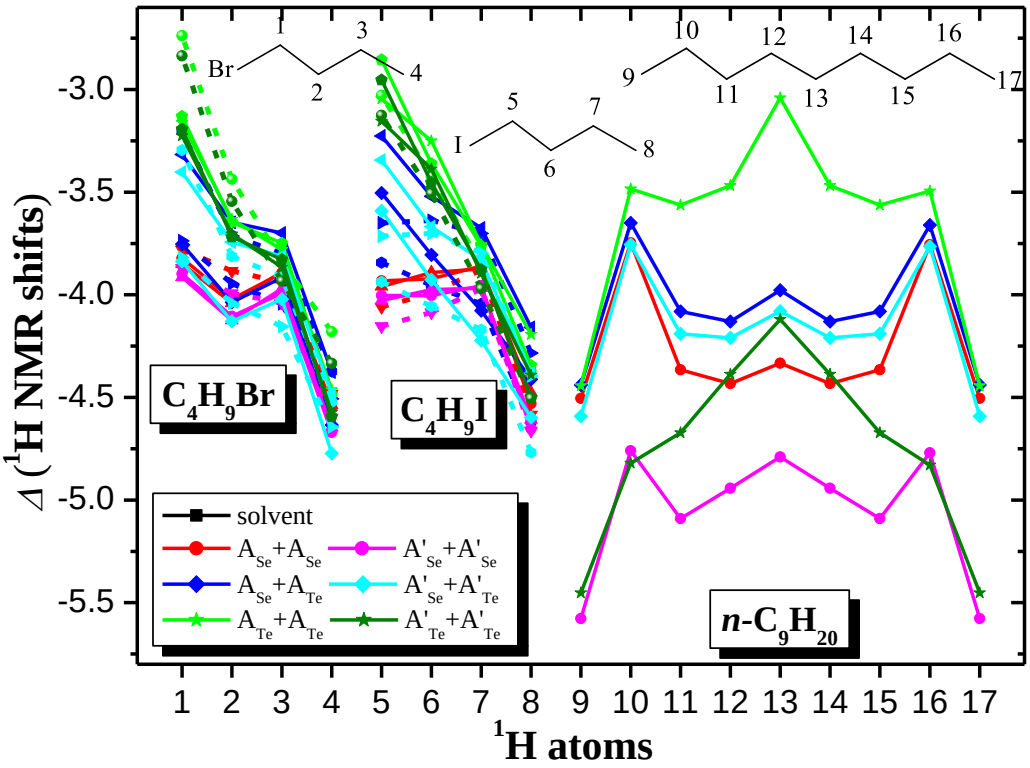
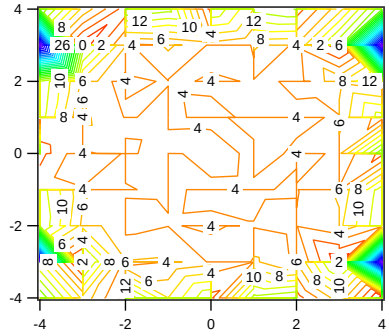
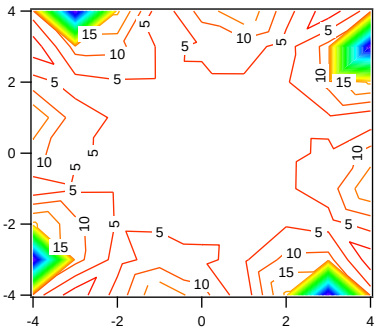
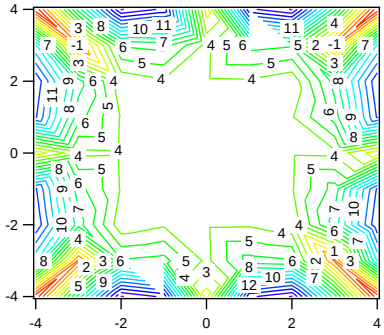
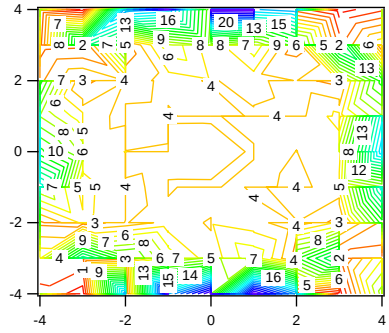
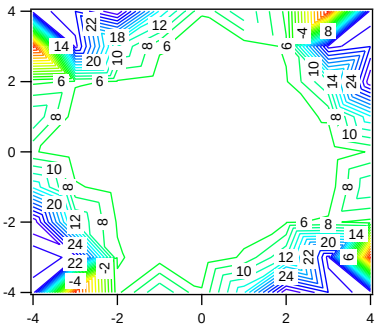
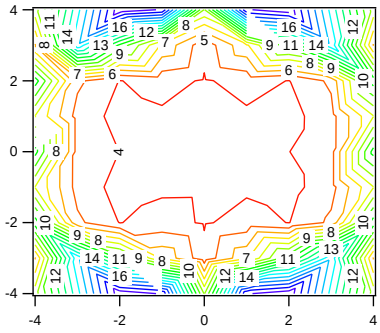
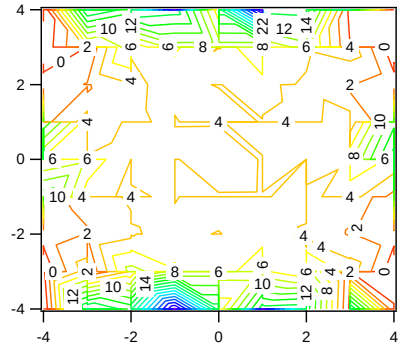
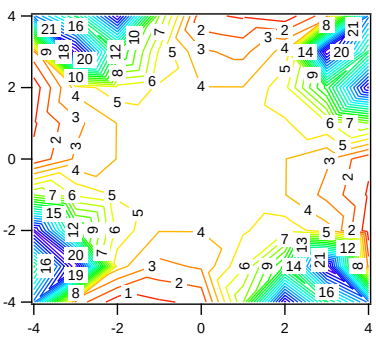
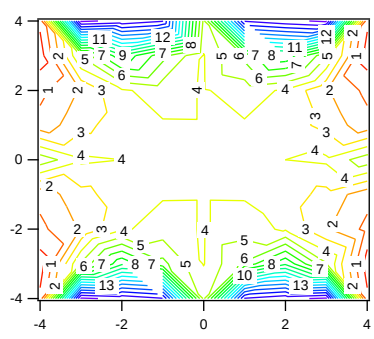
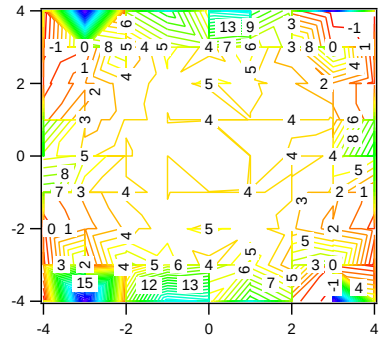
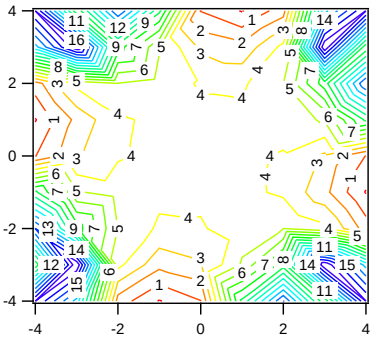
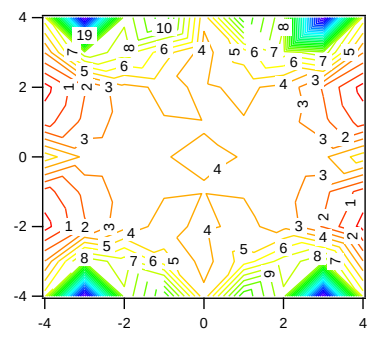
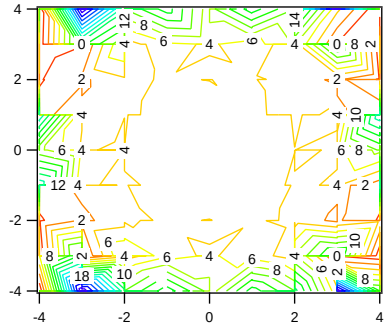
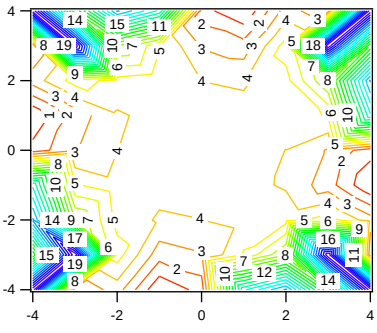
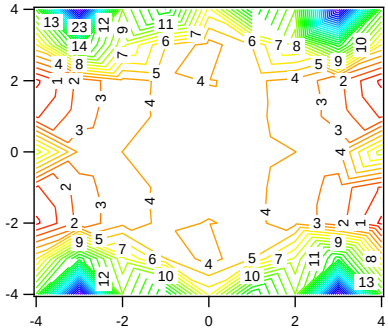


Figure 20S. Relative shifts of ^{1}H NMR shifts (ppm) of the 1-C_4H_9Br, 1-C_4H_9I and *n*-C_9H_{20} encapsulated compounds with respect to the free compounds at M06-2X/6-31G(d,p). Average ^{1}H NMR for the same C and for the symmetric C atoms; A(R=CH_3); A′(R=$CH_2CH_2CH_2Cl$).

R	A_{Se}+ A_{Se}	A_{Se}+ A_{Te}	A_{Te}+ A_{Te}
0			
1			
2			
3			
4			

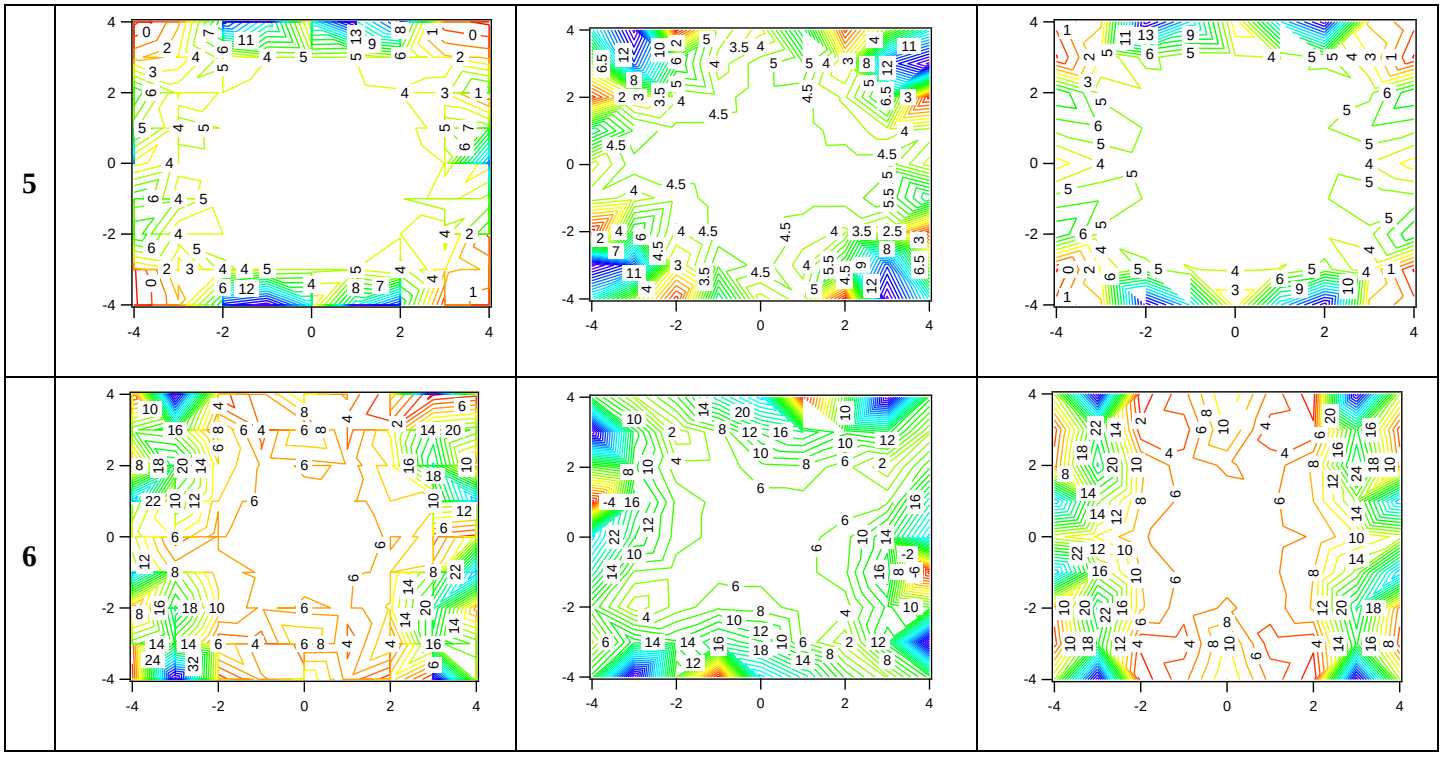
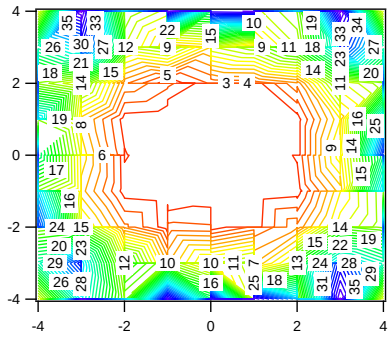
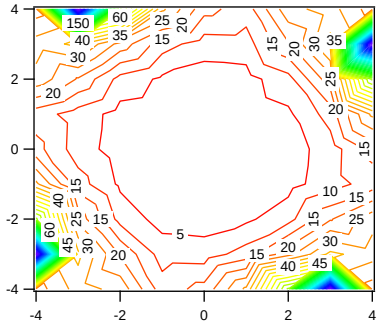
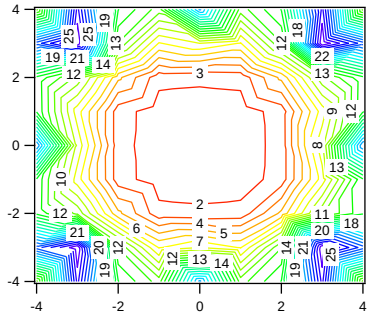
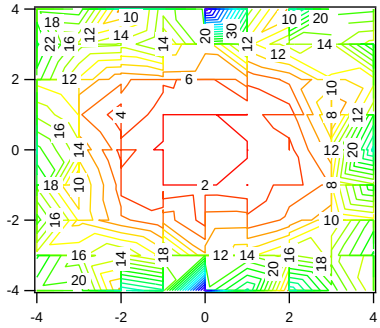
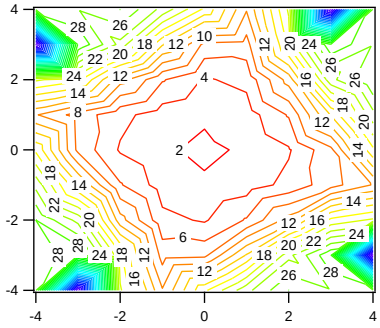
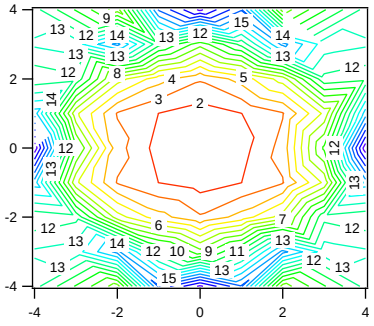
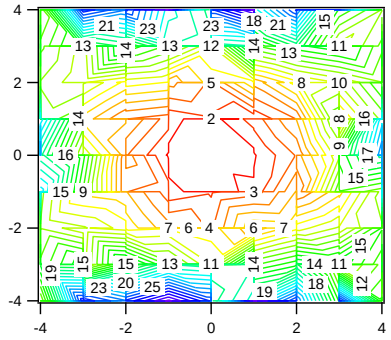
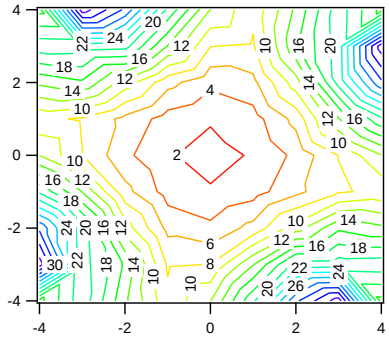
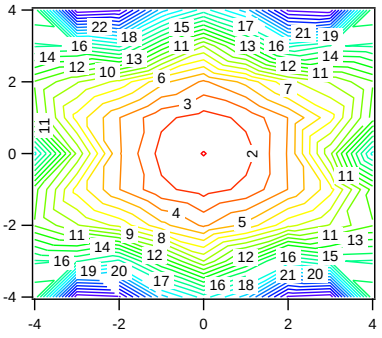
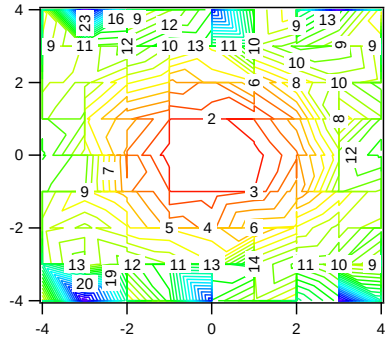
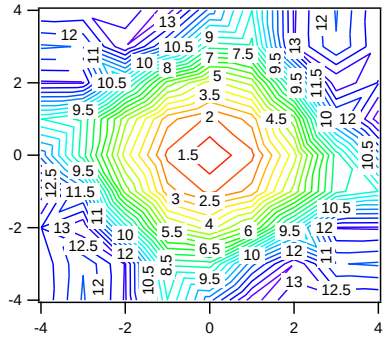
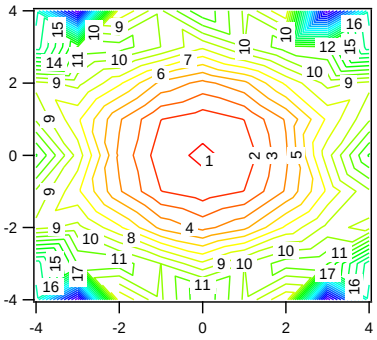
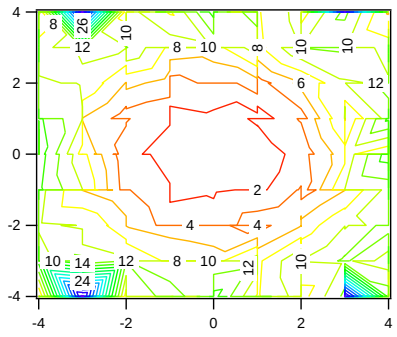
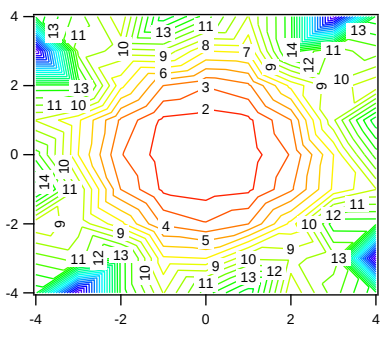
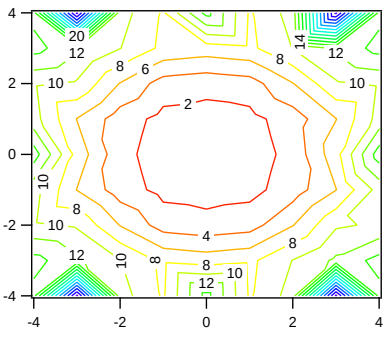


Figure 21S. Magnetic isotropy of $\mathbf{A_X + A_X}$ complexes, where X = O, S, Se and Te. Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.

R	$A_{Se}+A_{Se}$	$A_{Se}+A_{Te}$	$A_{Te}+A_{Te}$
0			
1			
2			
3			
4			

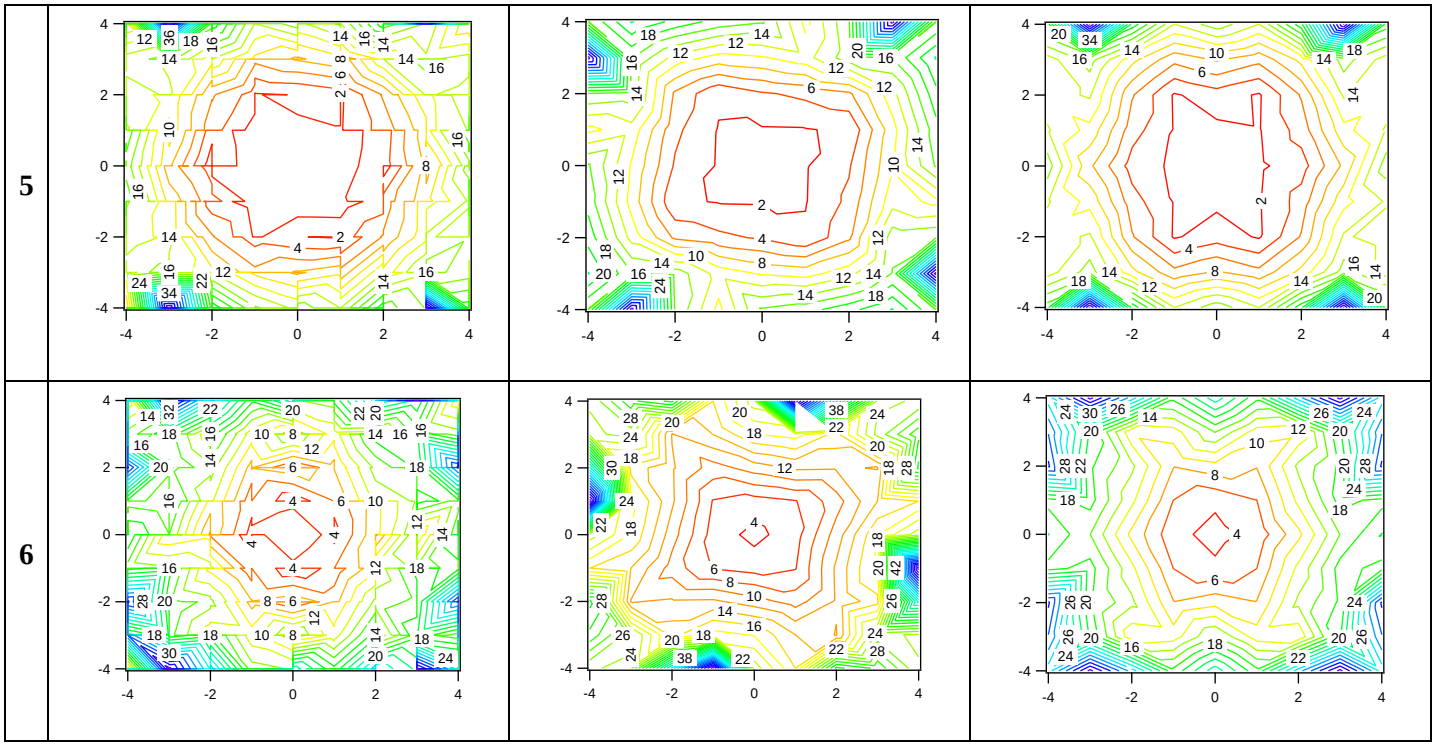
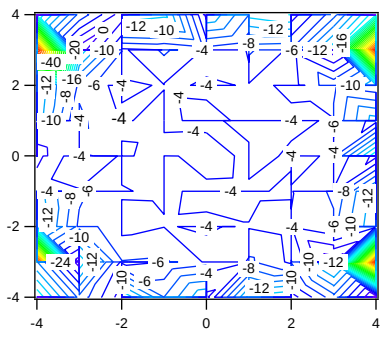
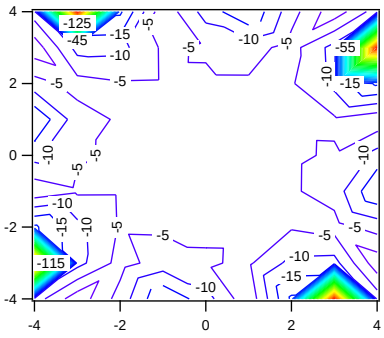
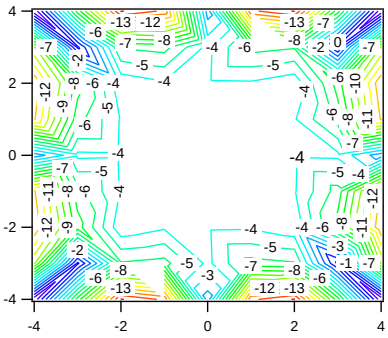
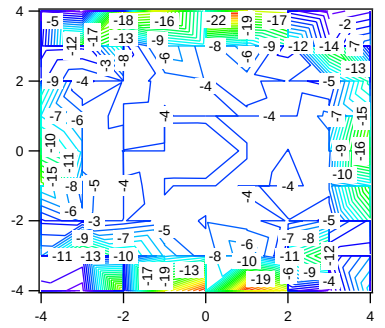
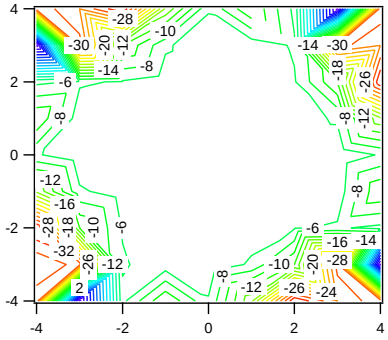
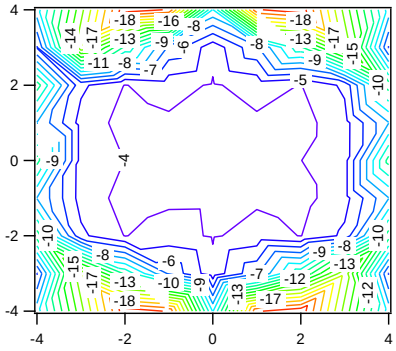
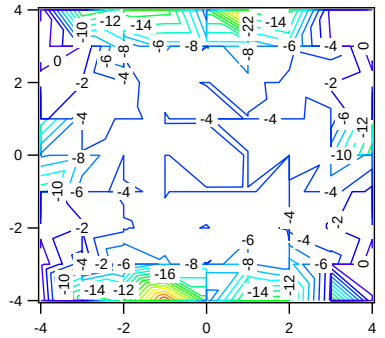
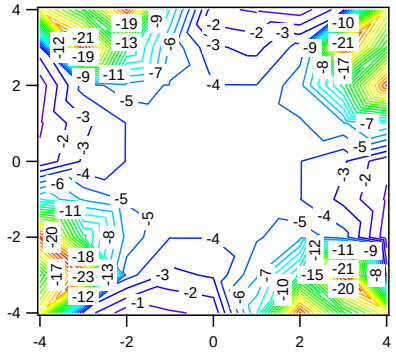
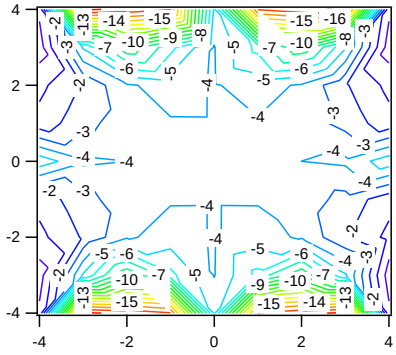
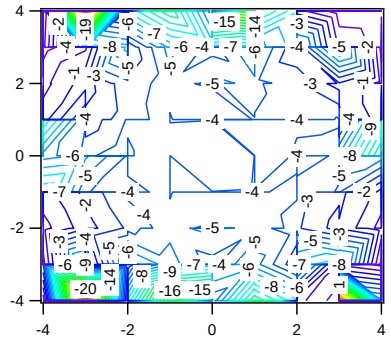
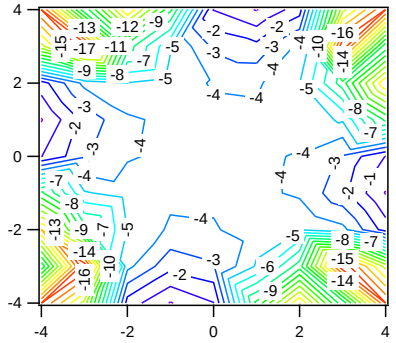
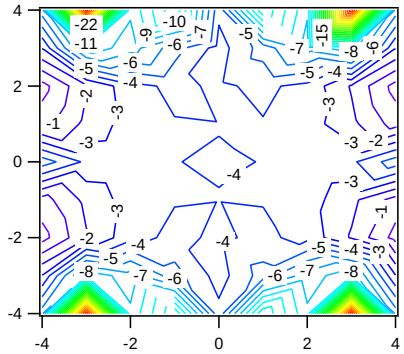
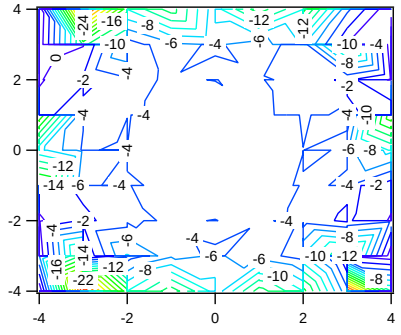
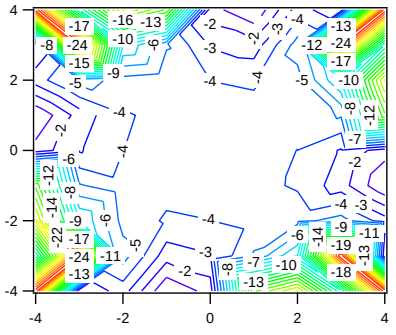
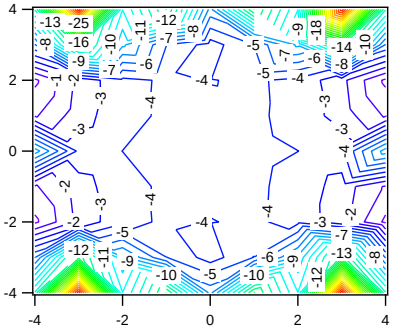


Figure 22S. Magnetic anisotropy of $\mathbf{A_X + A_X}$ complexes, where X = O, S, Se and Te. Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage

R	$A_{Se}+A_{Se}$	$A_{Se}+A_{Te}$	$A_{Te}+A_{Te}$
0			
1			
2			
3			
4			

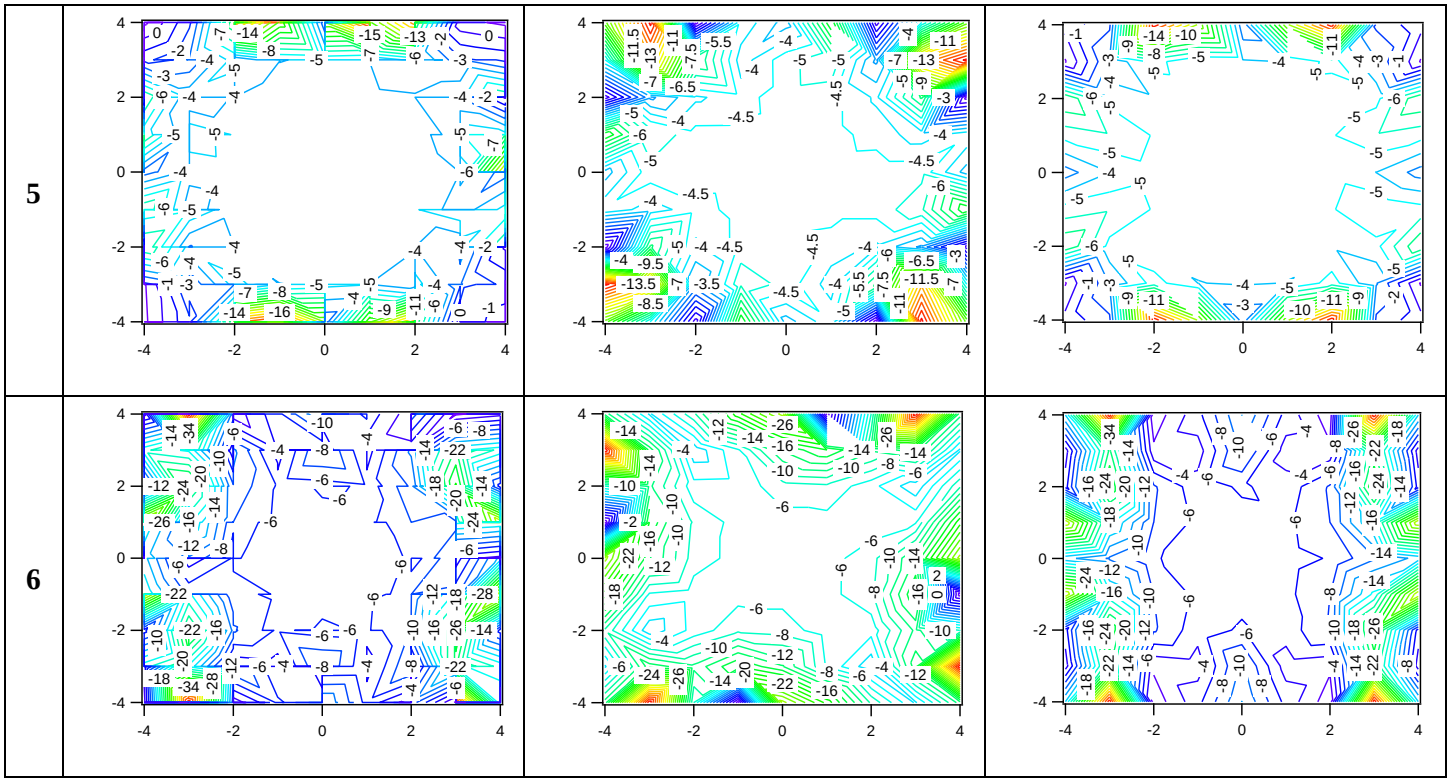


Figure 23S. NICS aromaticity indexes of $\mathbf{A_X}$+ $\mathbf{A_X}$ complexes, where X = O, S, Se and Te. Contour on the XY plane at distances R from the center of the cage along the main Z axis of the cage.

Experimental Section

All analytical grade solvents and reagents purchased from commercial sources were used without further purification. SeO_2 was purchased from Energy Chemical Company Ltd., Shanghai China. D_2O was used as NMR analysis solvents. ^1H and ^{13}C NMR analyses were performed using Bruker AVANCE III HD 600 MHz spectrophotometer. Positive ions high-resolution mass analyses were performed on Bruker micrOTOF II machine. Cavitand 1 was prepared using our previously reported protocol.[1]

^1H NMR spectra of 1 in water showing assembly with cyclic ketone

General procedure for the binding analyses

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and excess pure cyclic ketone (~0.5 µL or ~0.5 mg) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^1H NMR spectroscopy at rt.

^1H NMR spectra of 1 in water in the presence of different alkyl halides

General procedure for the binding analyses

1 mM, 0.5 mL of **1** in D_2O was taken in NMR tube and excess pure alkyl halide (~0.5 µL or ~0.5 mg) was added to the tube, it was shaken well to mix the guest in water. The sample was sonicated for 1 h at rt and analyzed by ^1H NMR spectroscopy at rt.

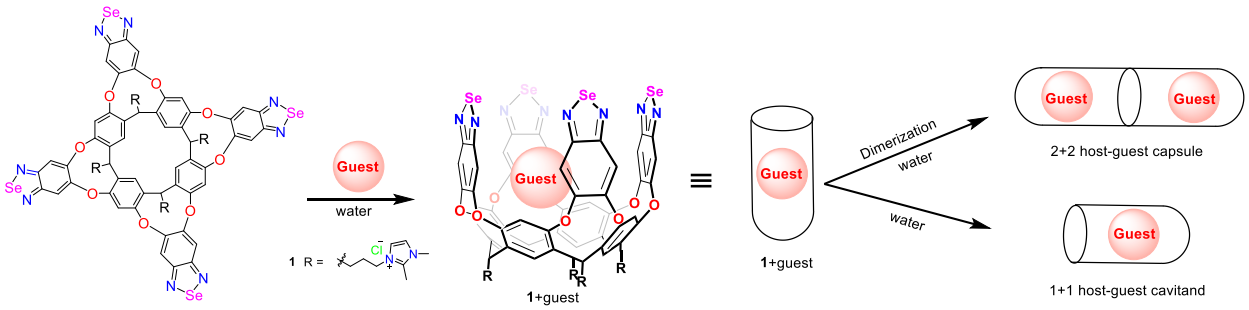


Fig. 24S Cartoons of 1 + 1 Host−Guest Cavitand and 2 + 2 and 2 + 1 Host−Guest Capsules

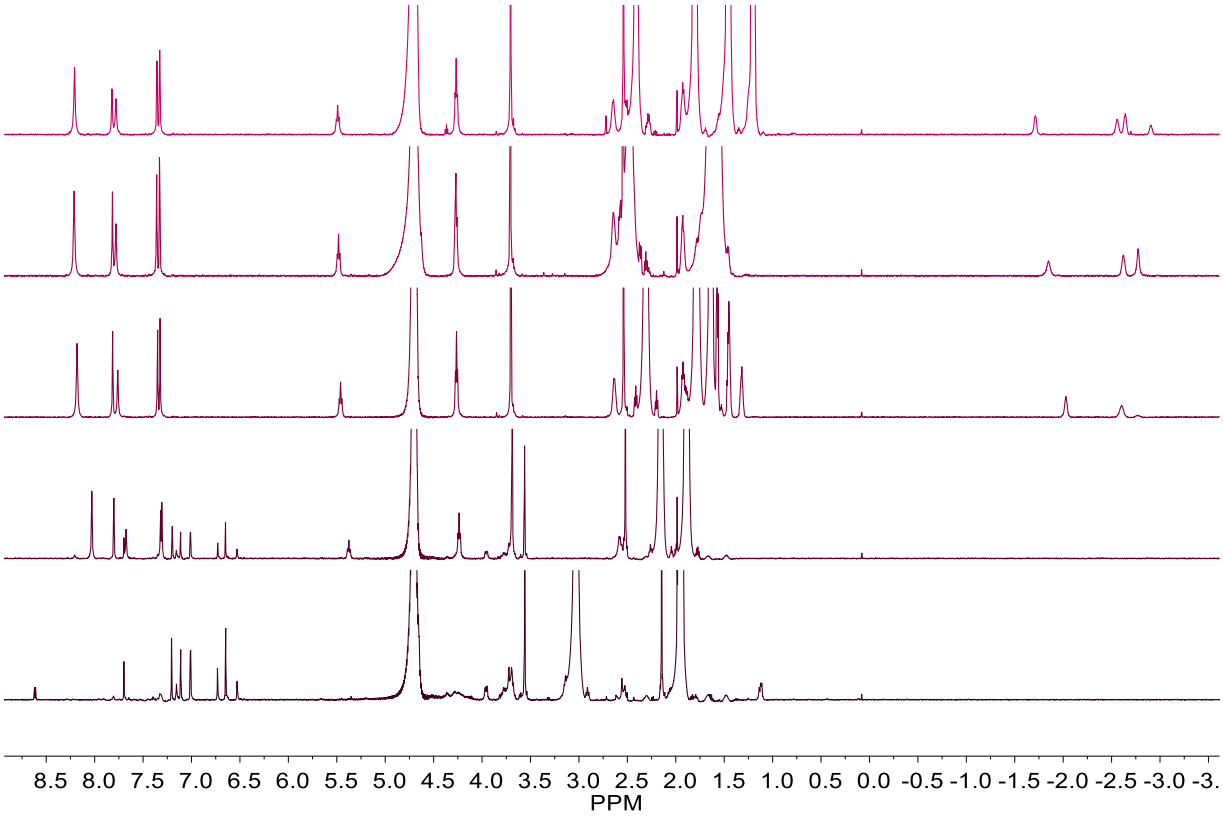


Fig. 25S ^{1}H NMR spectrum of the complex formed between **1** + cycloketone in D_2O (600 MHz, rt) from bottom to top, cyclobutanone, cyclopentanone, cyclohexanone, cycloheptanone, cyclooctenone

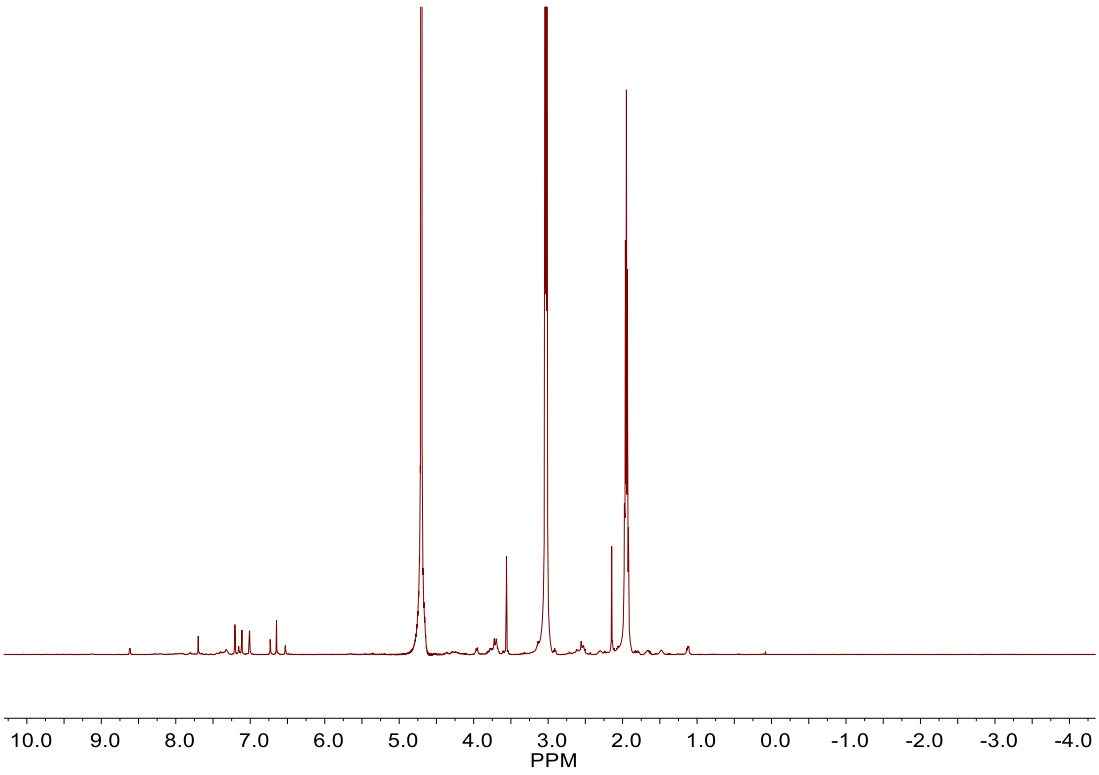


Fig. 26S ^{1}H NMR spectrum of the complex formed between **1** + cyclobutanone in D_2O (600 MHz, rt)

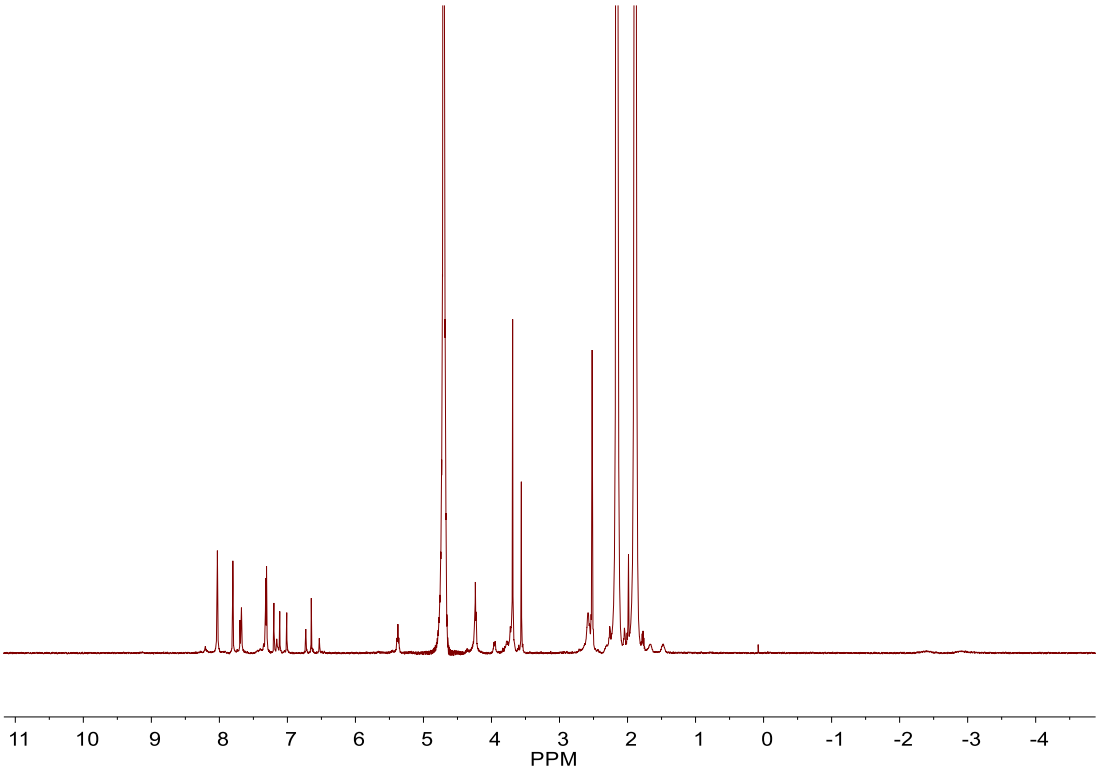


Fig. 27S ^{1}H NMR spectrum of the complex formed between **1** + cyclopentanone in D_2O (600 MHz, rt)

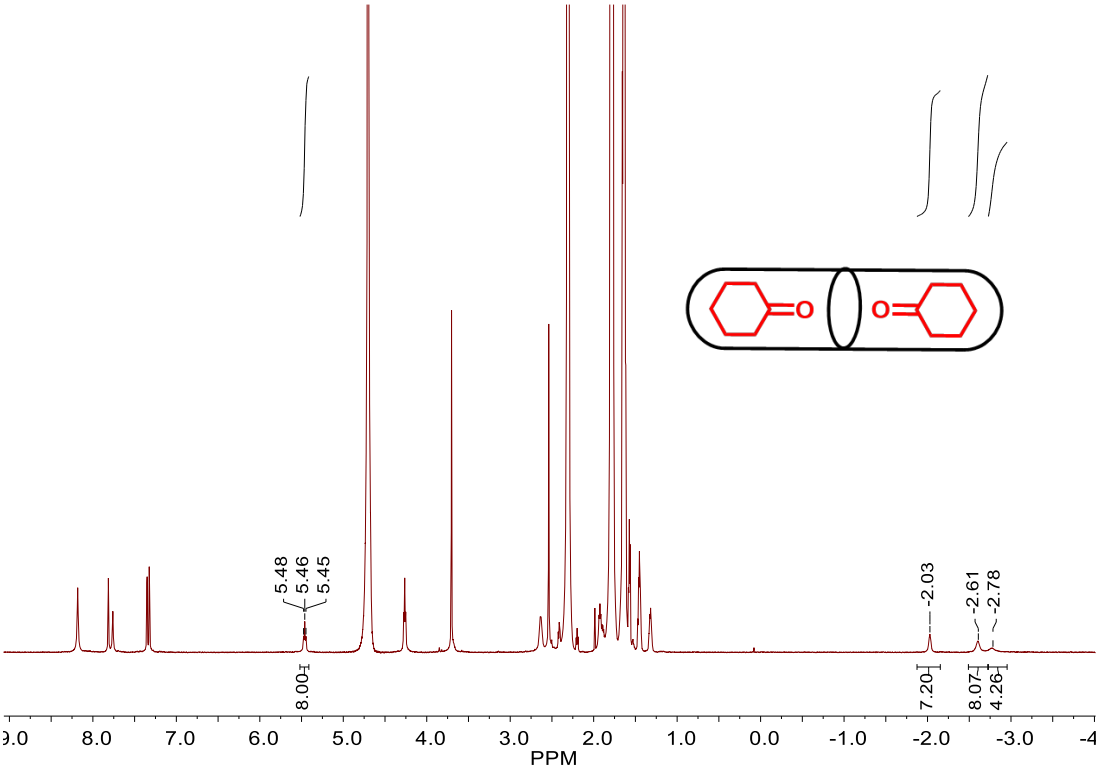


Fig. 28S ^{1}H NMR spectrum of the complex formed between **1** + cyclohexanone in D_2O (600 MHz, rt)

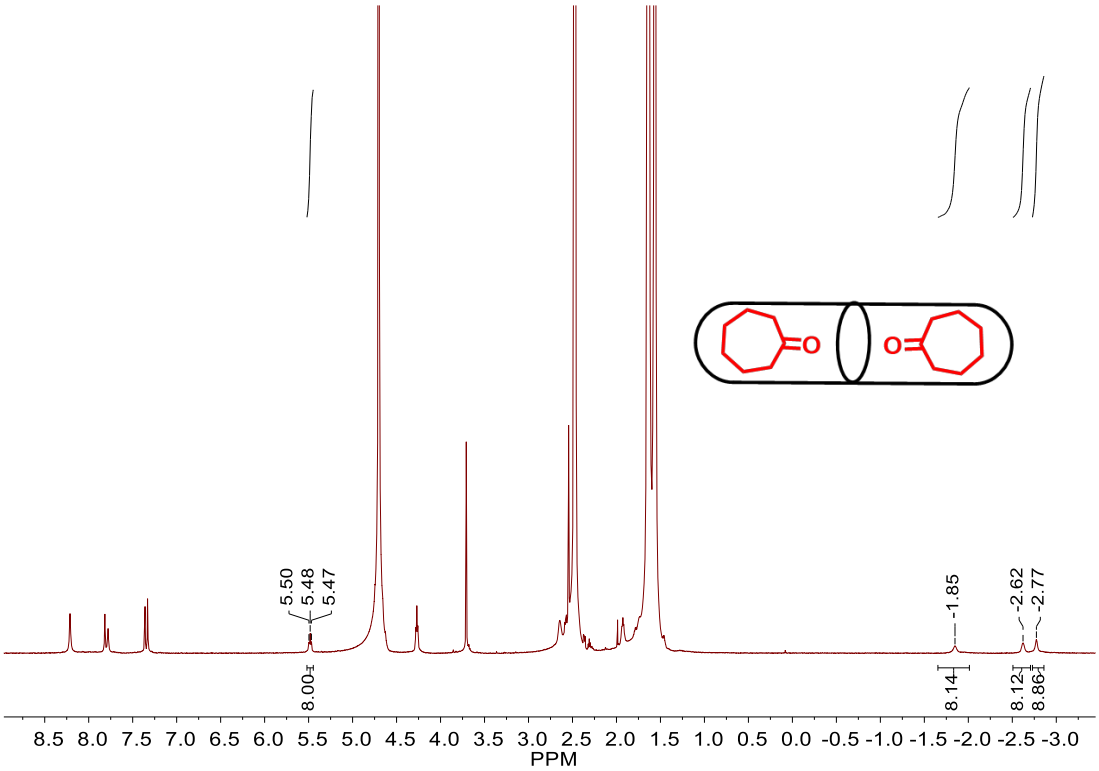


Fig. 29S ^{1}H NMR spectrum of the complex formed between **1** + cycloheptanone in D_2O (600 MHz, rt)

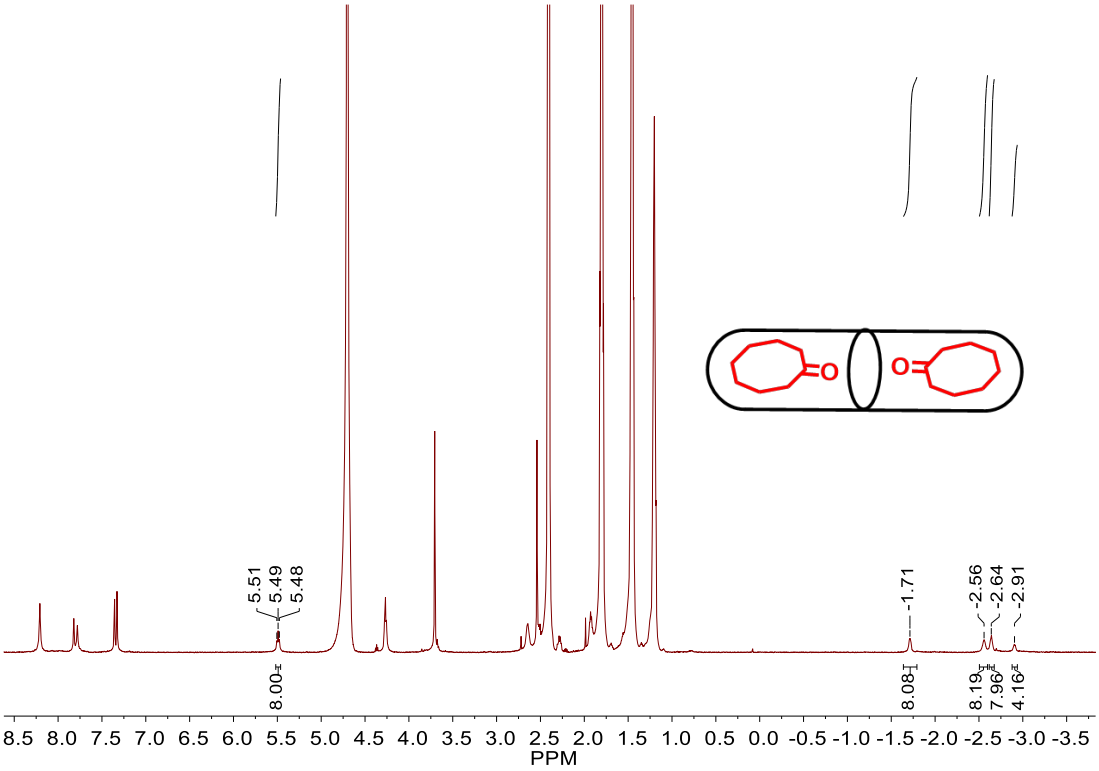


Fig. 30S ^{1}H NMR spectrum of the complex formed between **1** + cyclooctanone in D_2O (600 MHz, rt)

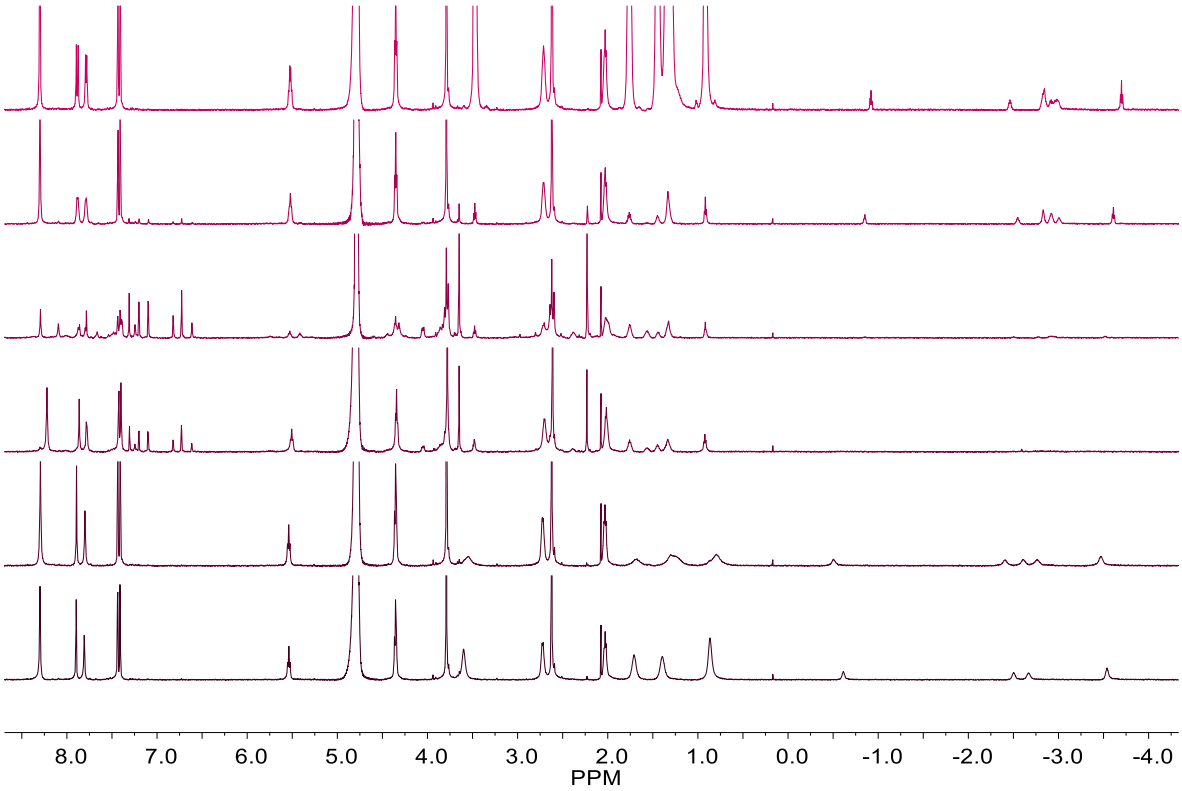


Fig. 31S ^{1}H NMR spectrum of the complex formed between **1** + 1-chloroalkane in D_2O (600 MHz, rt) from bottom to top, 1-chlorobutane, 1-chloropentane, 1-chlorohexane, 1-chloroheptane, 1-chlorooctane, 1-chlorononane

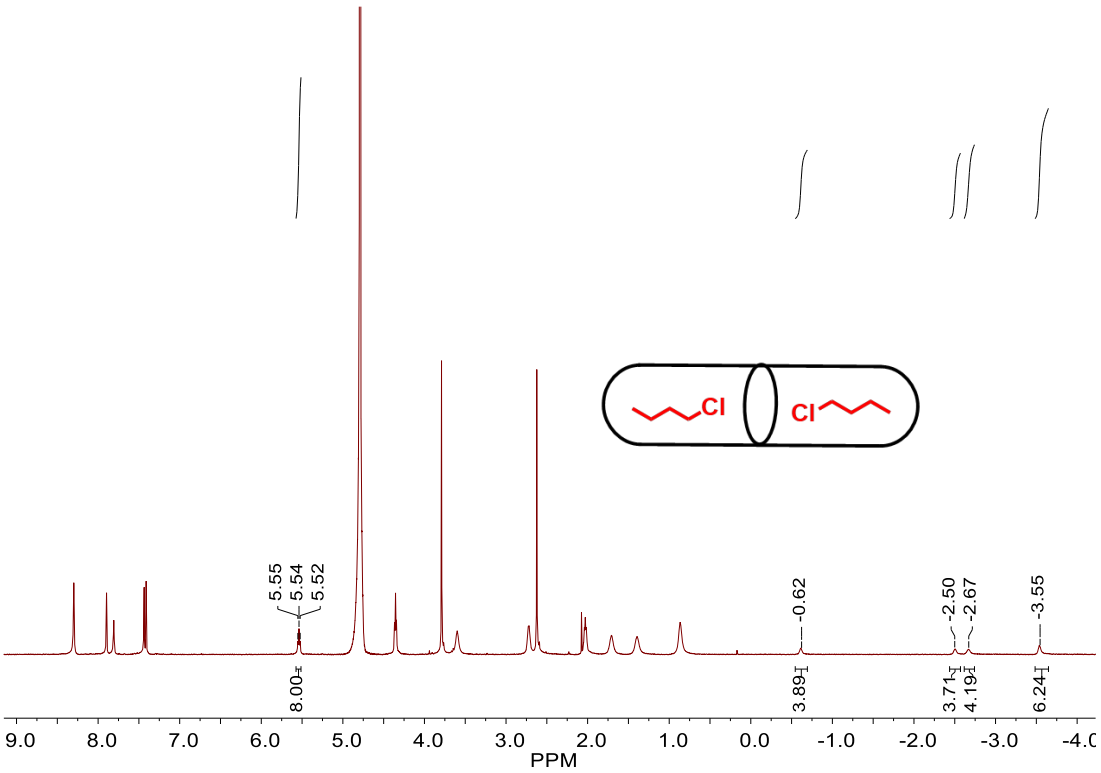


Fig. 32S ^{1}H NMR spectrum of the complex formed between **1** + 1-chlorobutane in D_2O (600 MHz, rt)

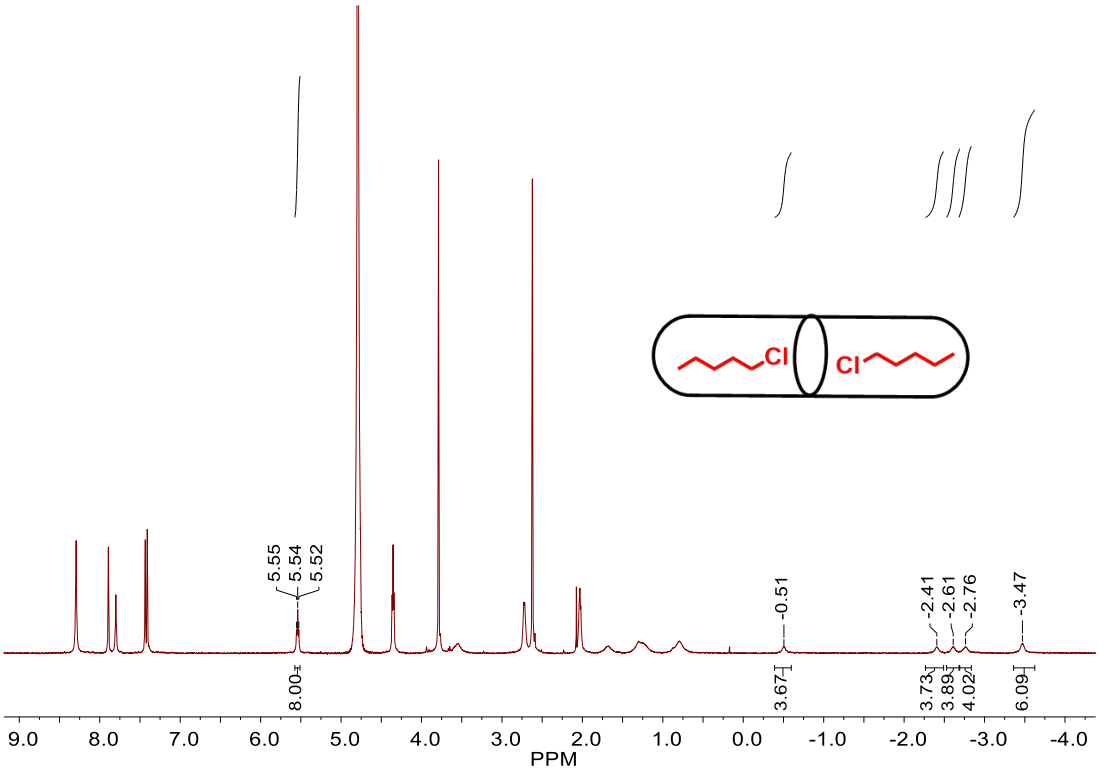


Fig. 33S ^{1}H NMR spectrum of the complex formed between **1** + 1-chloropentane in D_2O (600 MHz, rt)

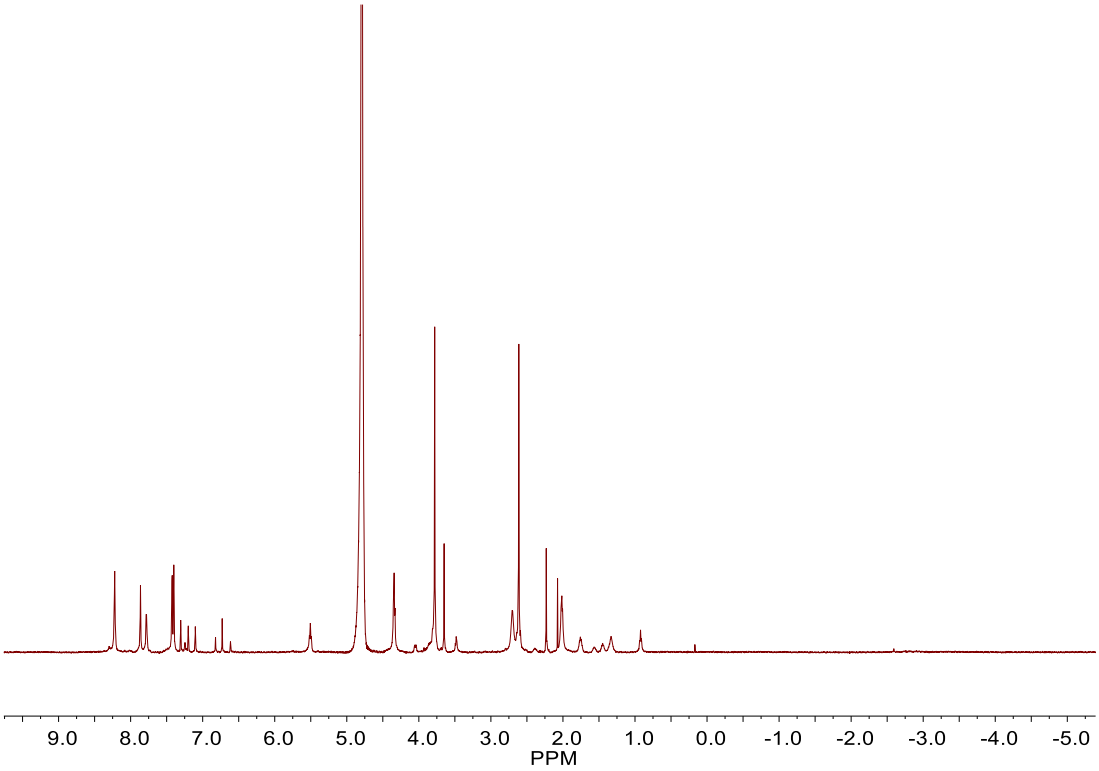


Fig. 14S ^{1}H NMR spectrum of the complex formed between **1** + 1-chlorohexane in D_2O (600 MHz, rt)

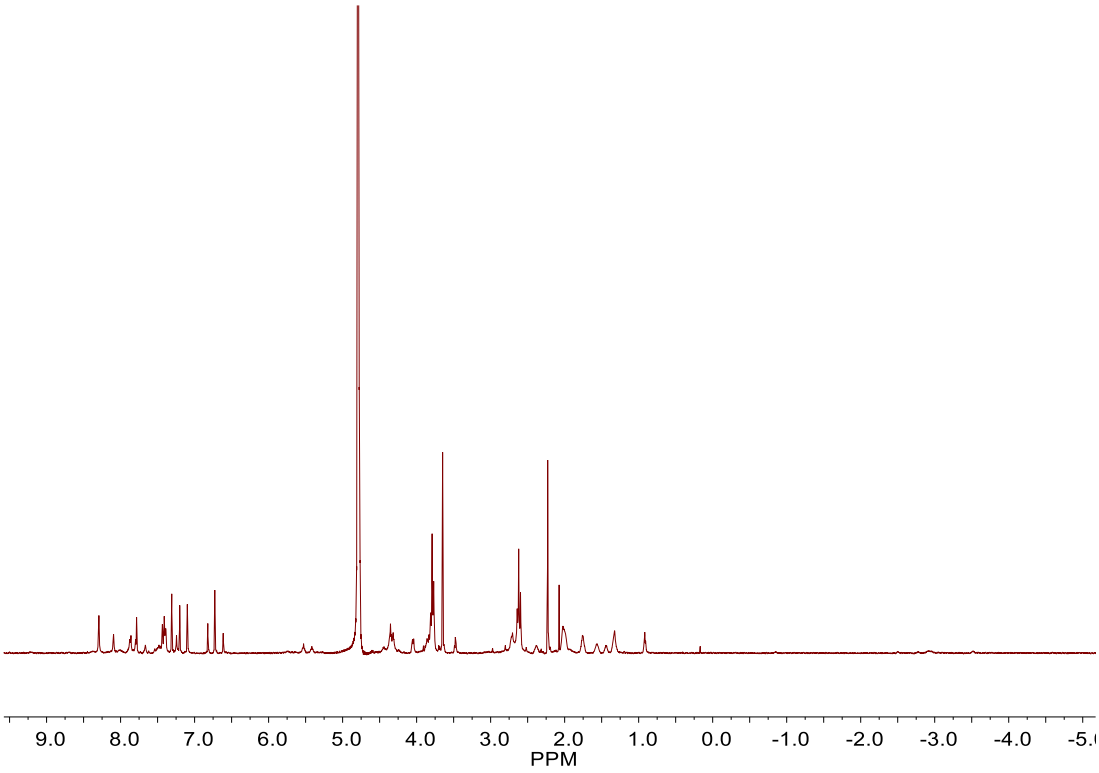


Fig. 35S [1]H NMR spectrum of the complex formed between **1** + 1-chloroheptane in D_2O (600 MHz, rt)

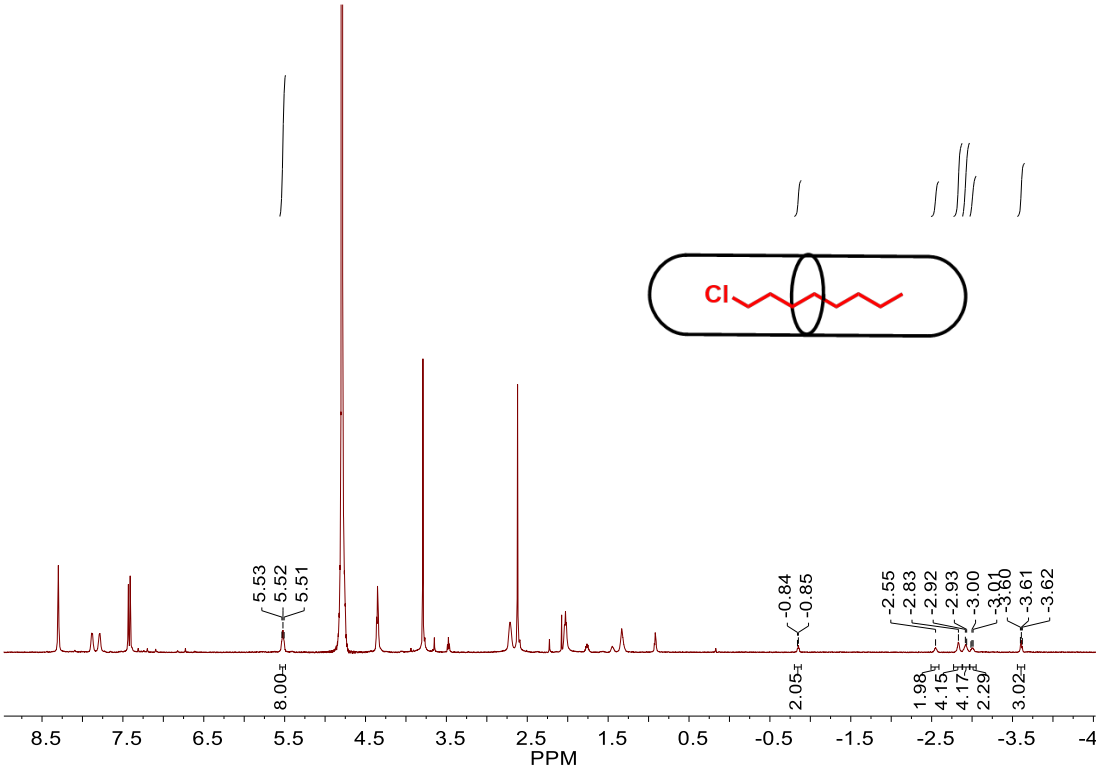


Fig. 362S [1]H NMR spectrum of the complex formed between **1** + 1-chlorooctane in D_2O (600 MHz, rt)

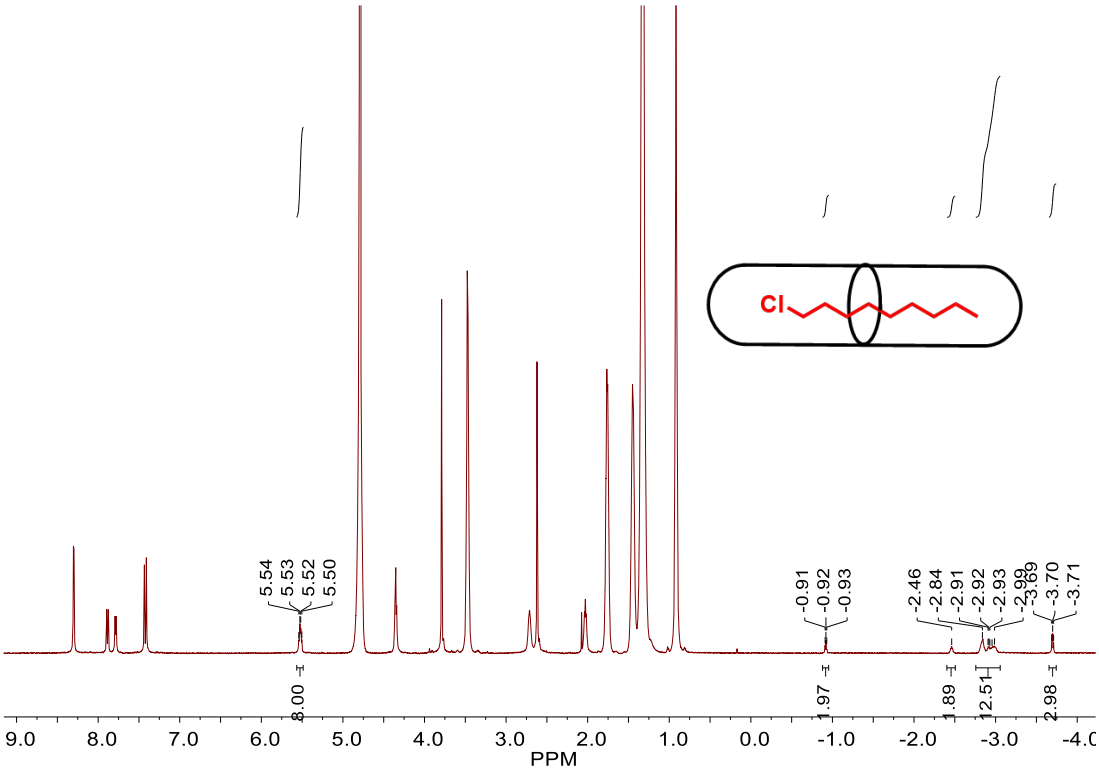


Fig. 37S ^{1}H NMR spectrum of the complex formed between **1** + 1-chlorononane in D_2O (600 MHz, rt)

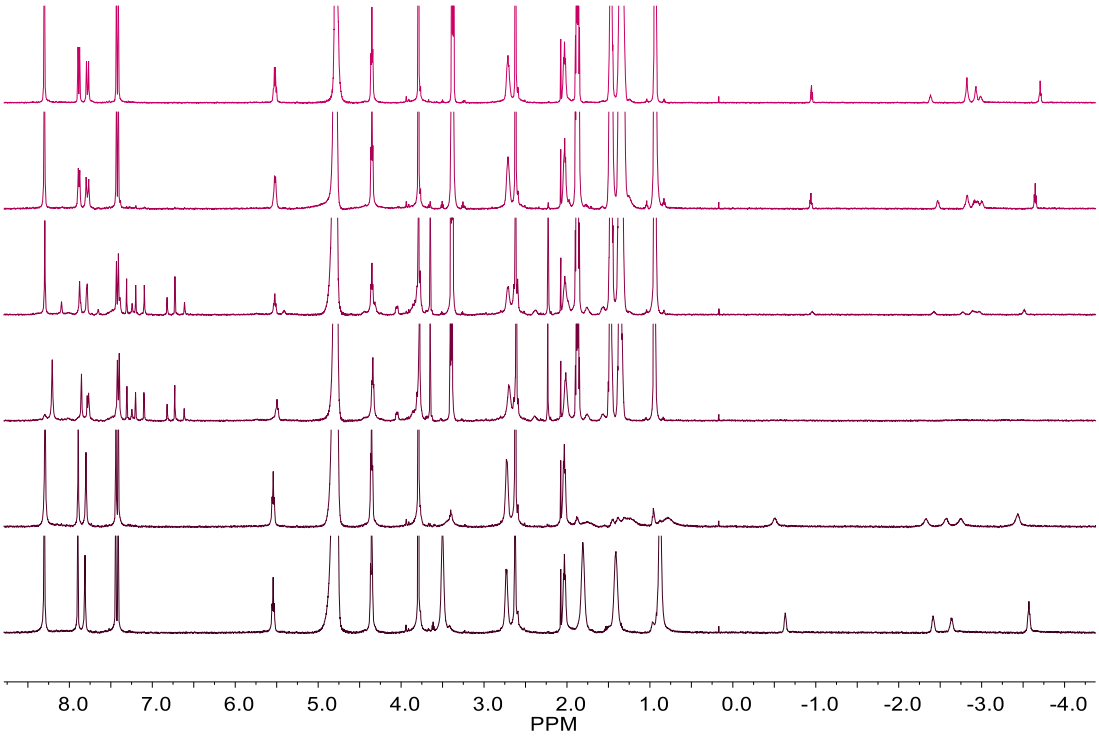


Fig. 38S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromoalkane in D_2O (600 MHz, rt) from bottom to top, 1-bromobutane, 1-bromopentane, 1-bromohexane, 1-bromoheptane, 1-bromooctane, 1-bromononane

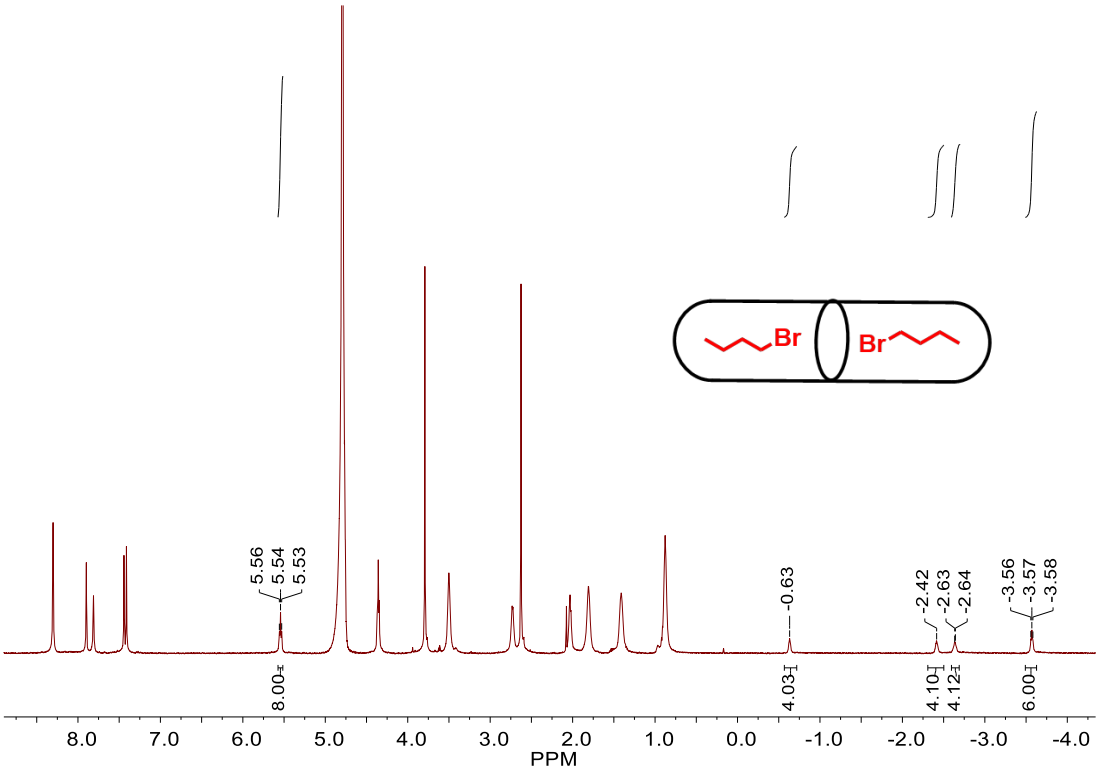


Fig. 39S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromobutane in D_2O (600 MHz, rt)

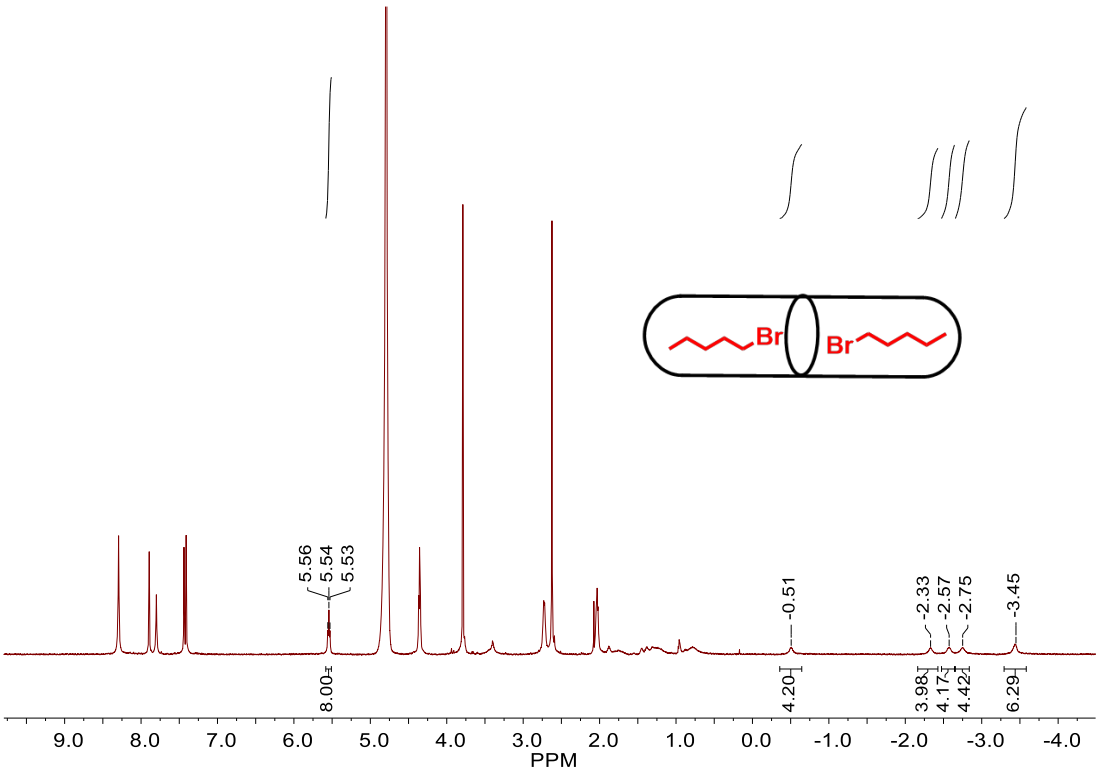


Fig. 40S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromopentane in D_2O (600 MHz, rt)

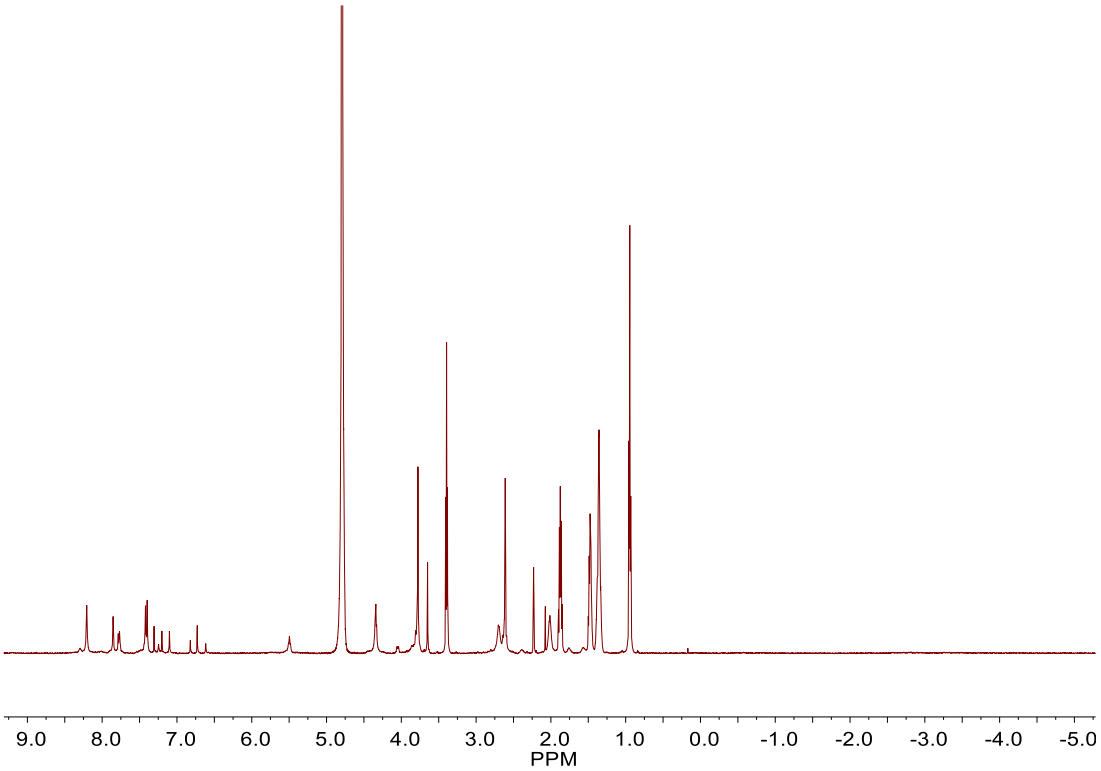


Fig. 41S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromohexane in D_2O (600 MHz, rt)

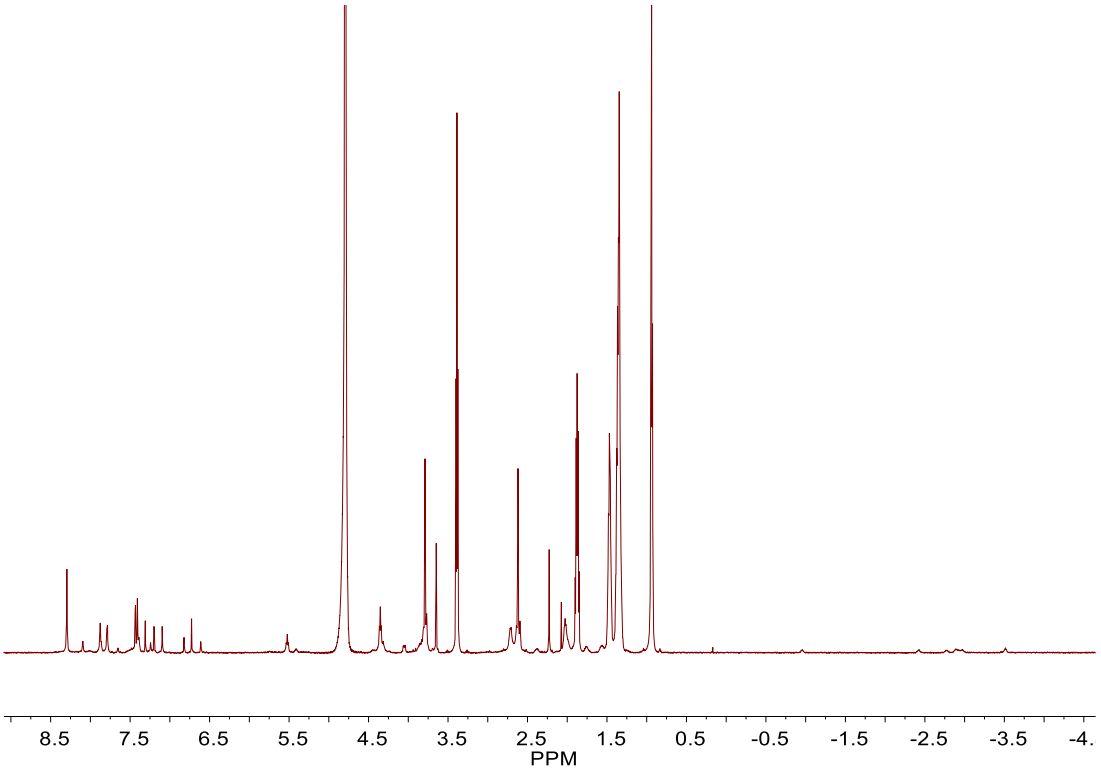


Fig. 42S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromoheptane in D_2O (600 MHz, rt)

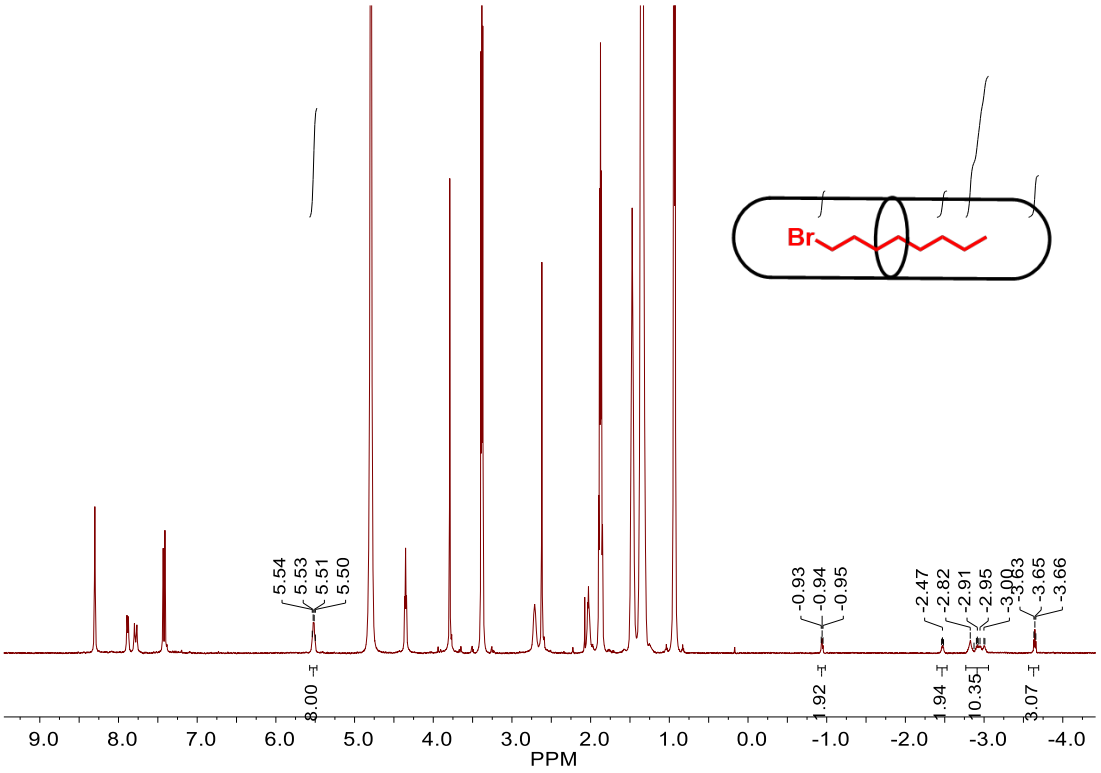


Fig. 43S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromooctane in D_2O (600 MHz, rt)

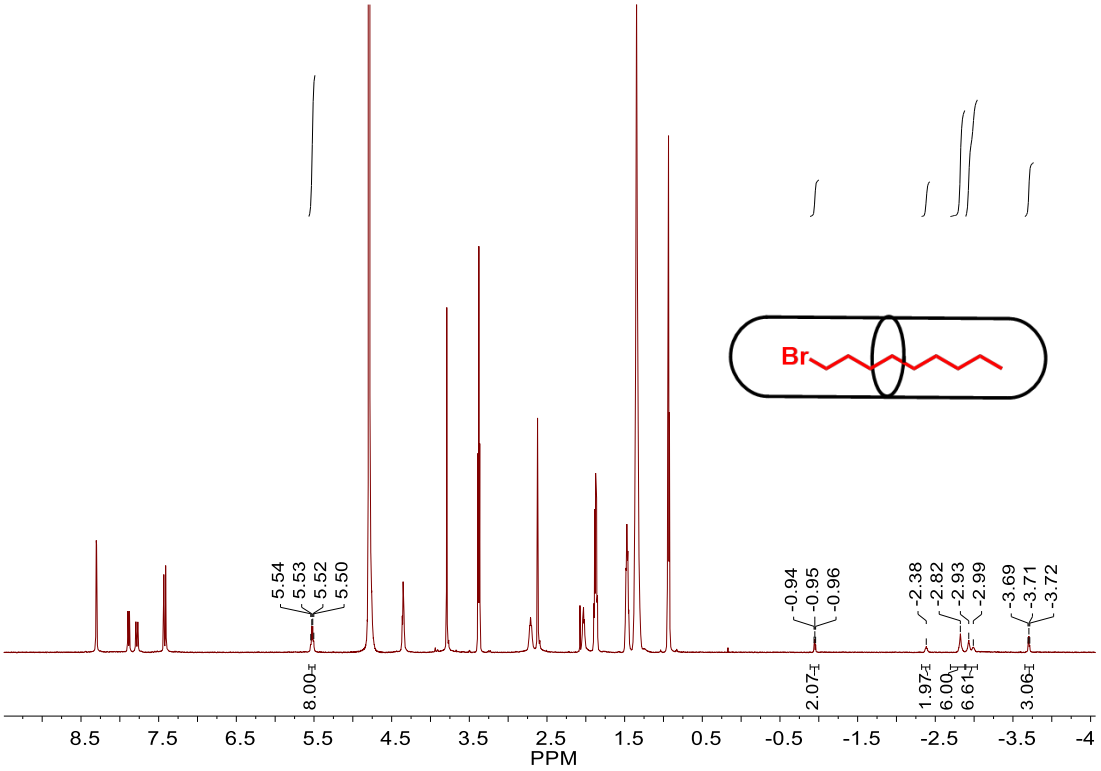


Fig. 44S ^{1}H NMR spectrum of the complex formed between **1** + 1-bromononane in D_2O (600 MHz, rt)

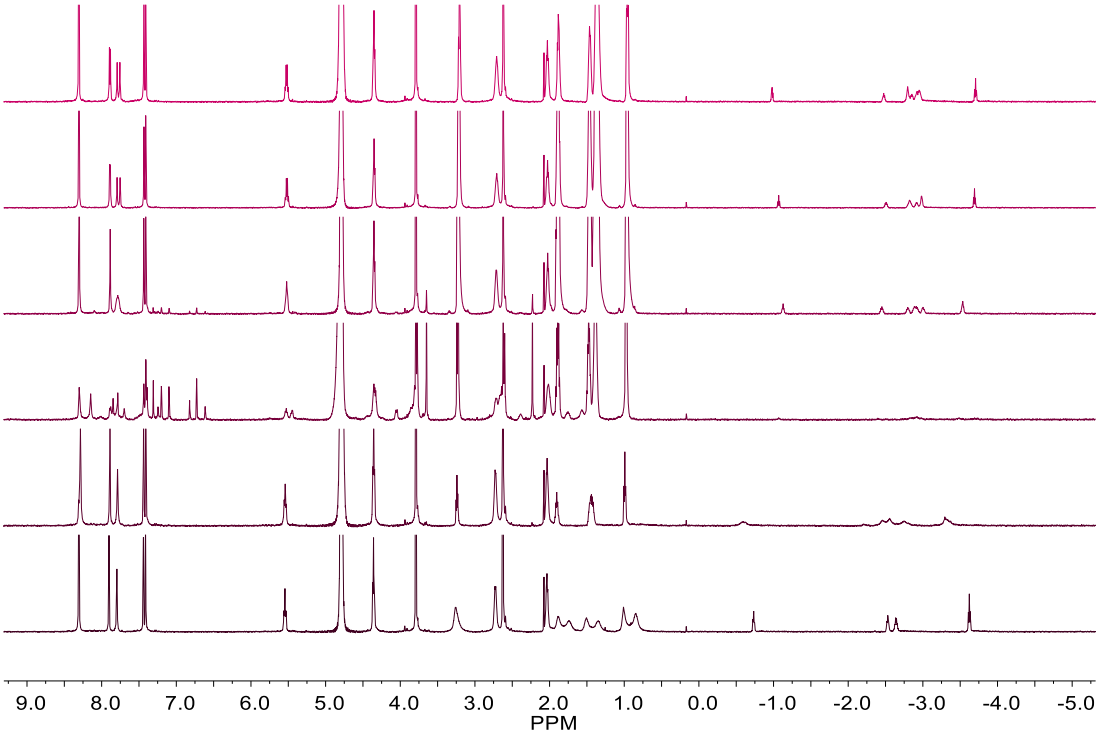


Fig. 45S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodoalkane in D_2O (600 MHz, rt) from bottom to top, 1-iodobutane, 1-iodopentane, 1-iodohexane, 1-iodoheptane, 1-iodooctane, 1-iodononane

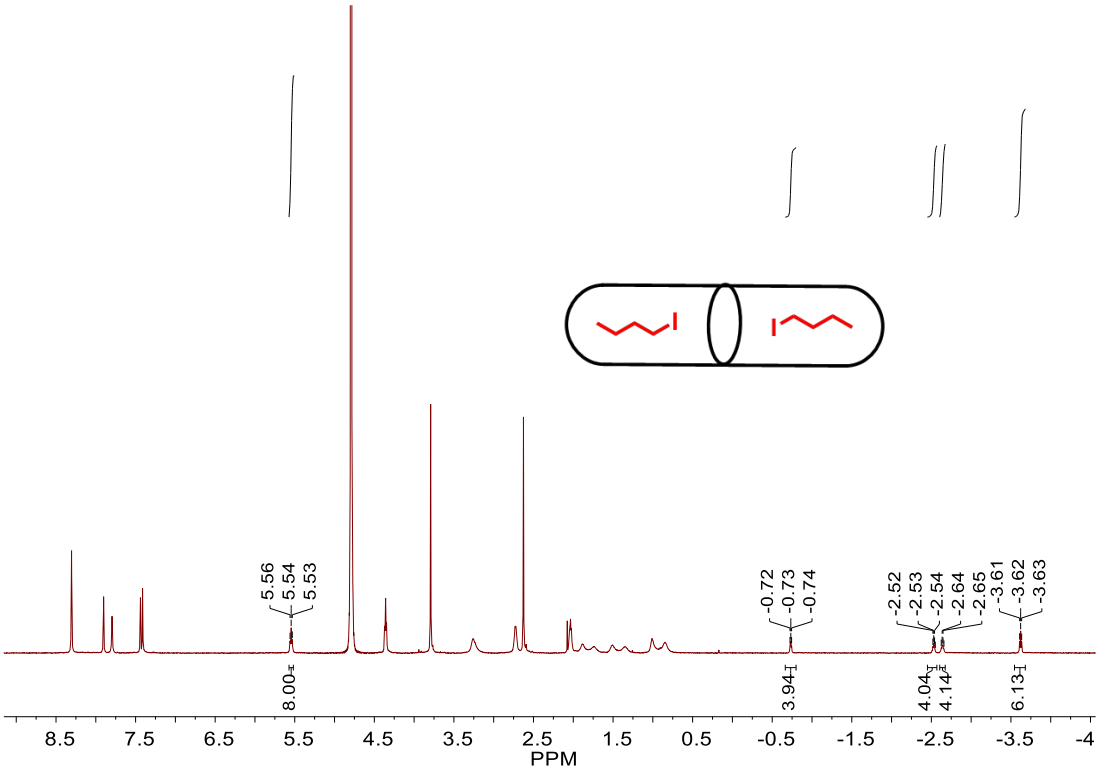


Fig. 46S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodobutane in D_2O (600 MHz, rt)

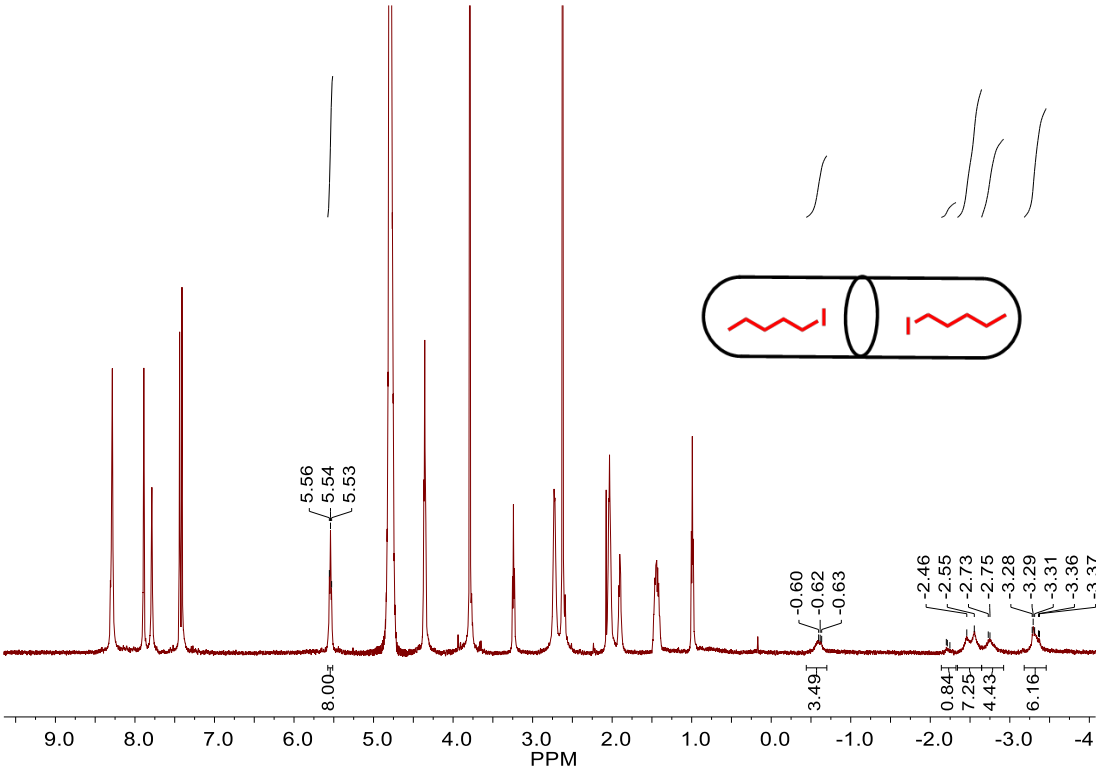


Fig. 47S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodopentane in D_2O (600 MHz, rt)

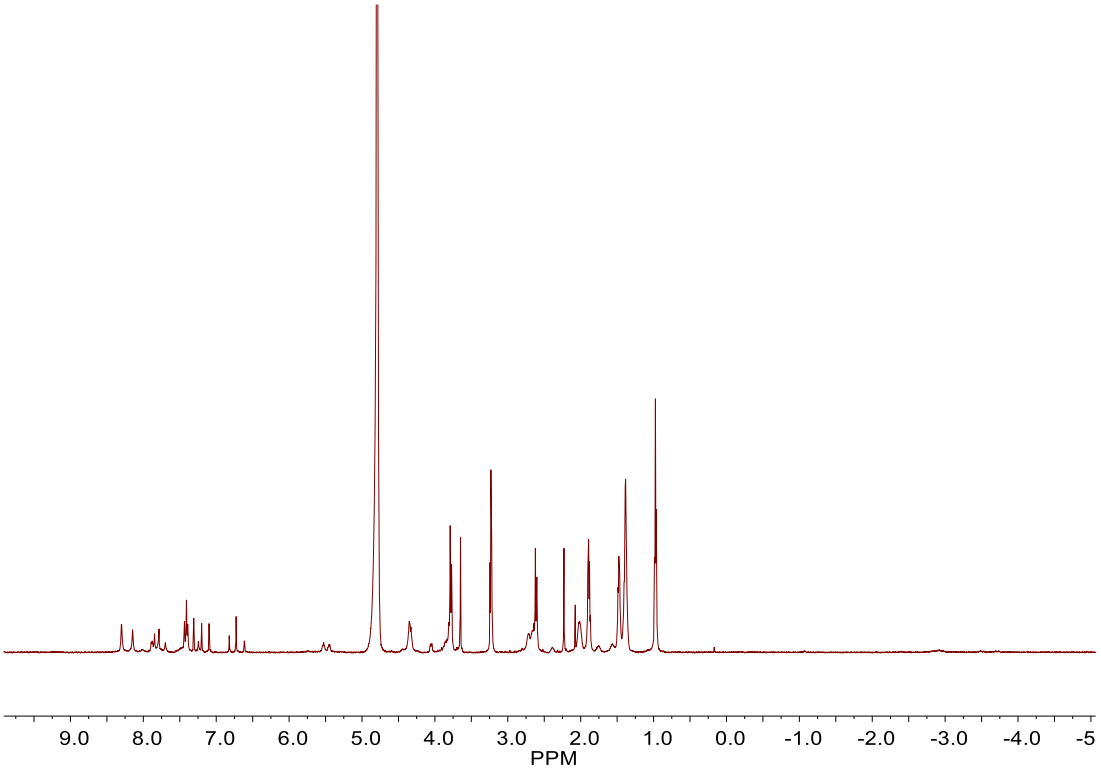


Fig. 48S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodohexane in D_2O (600 MHz, rt)

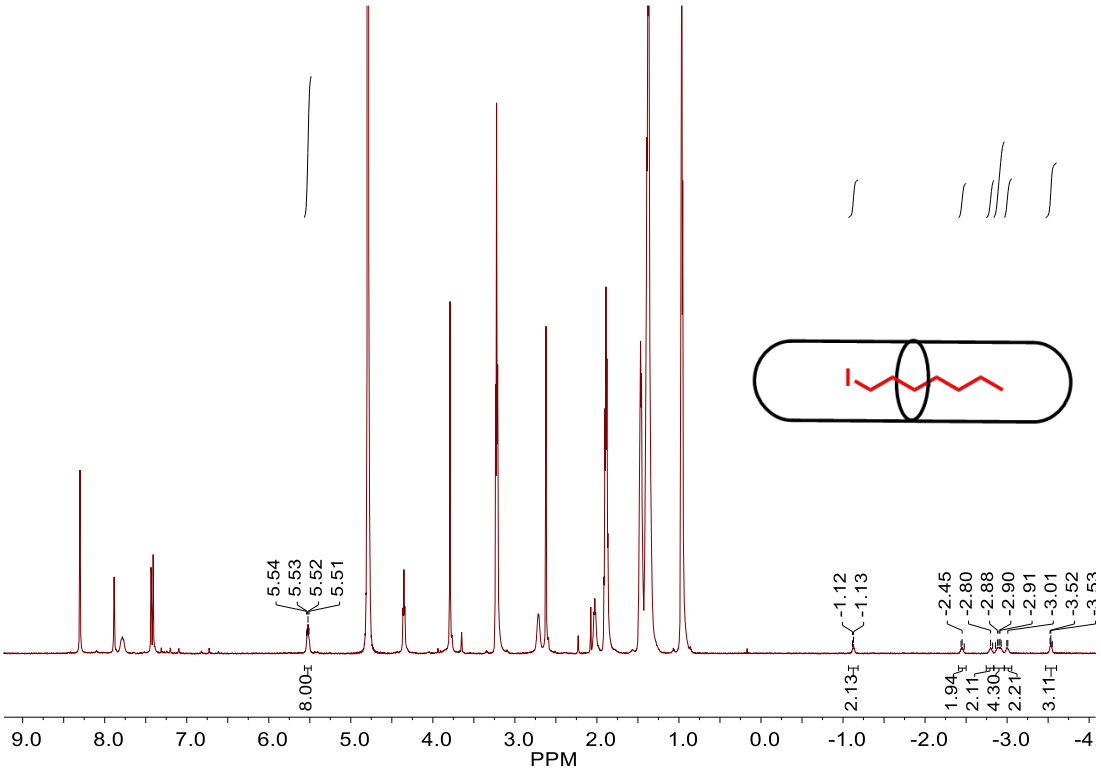


Fig. 49S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodoheptane in D_2O (600 MHz, rt)

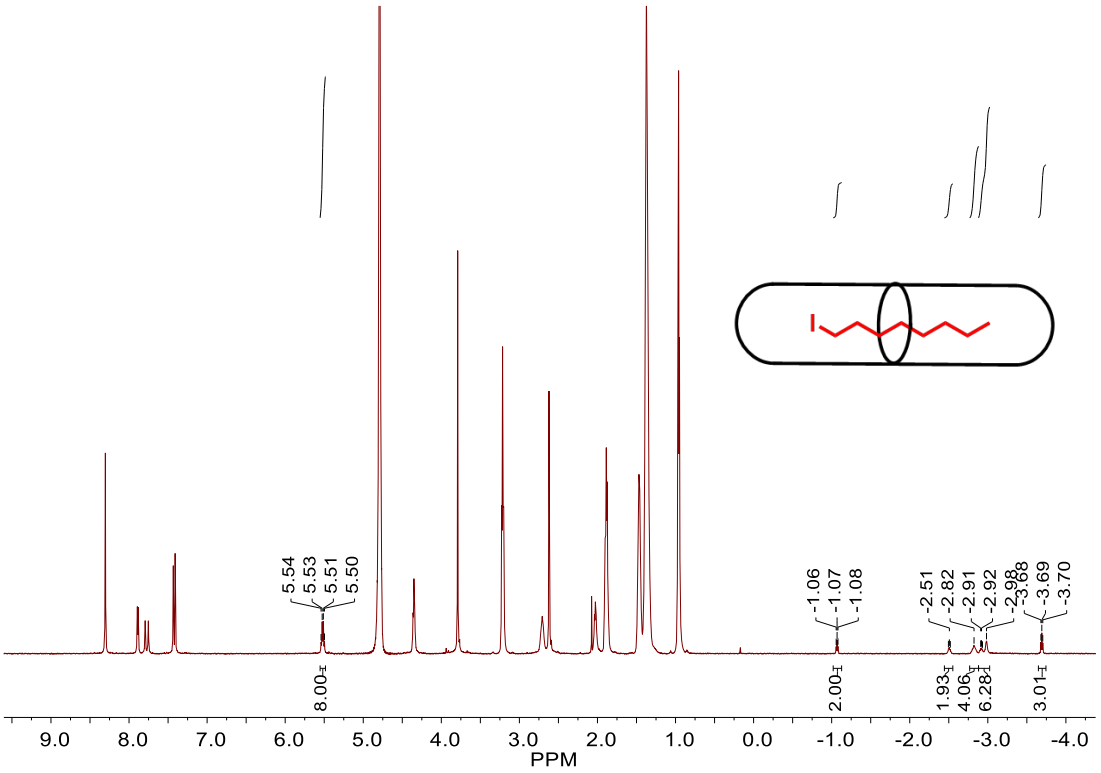


Fig. 50S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodooctane in D_2O (600 MHz, rt)

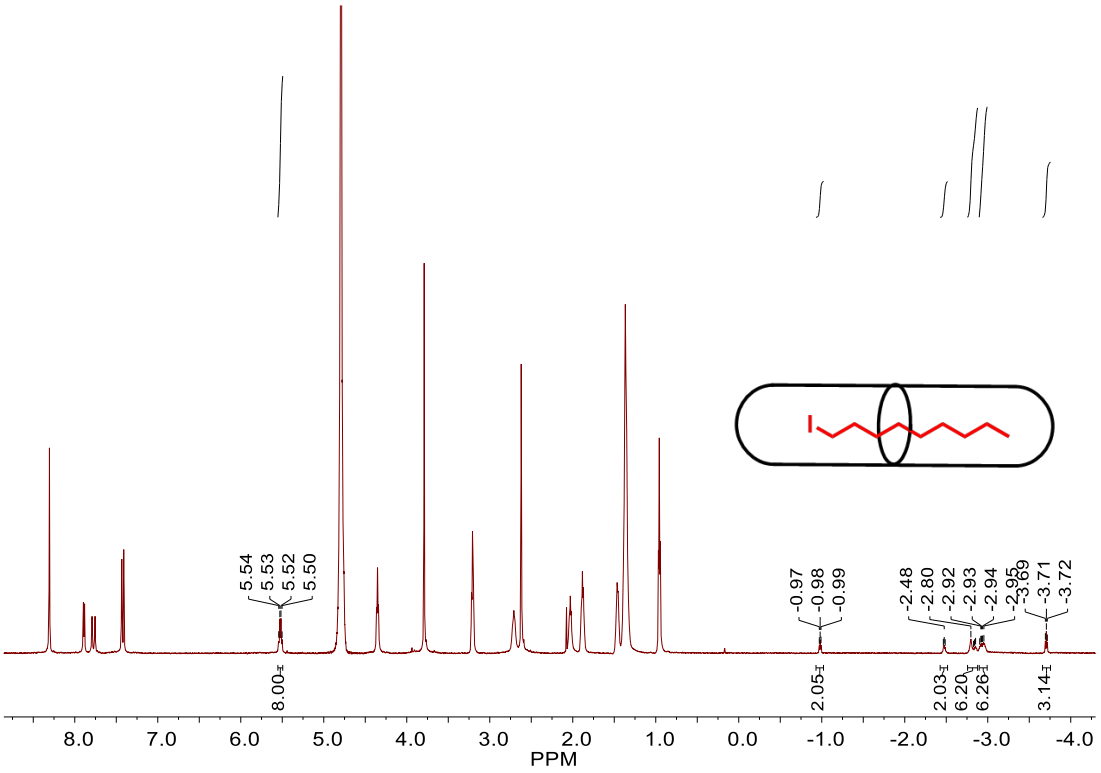


Fig. 51S ^{1}H NMR spectrum of the complex formed between **1** + 1-iodononane in D_2O (600 MHz, rt)

References

1. Rahman, F. U.; Tzeli, D.; Petsalakis, I. D.; Theodorakopoulos, G.; Ballester, P.; Rebek, J., Jr.; Yu, Y., Chalcogen Bonding and Hydrophobic Effects Force Molecules into Small Spaces. *J. Am. Chem. Soc.* **2020,** *142* (12), 5876-5883.