

## Supporting Information

# General AMBER Force Field Parameters for Diphenyl Diselenides and Diphenyl Ditellurides

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**Table S1.** Force-field parameters; values for Te analogue are given in brackets.<sup>a</sup> This is the factor which divides the barriers. <sup>b</sup> New parameters

(p-NH <sub>2</sub> -PhX) <sub>2</sub>									
bonds		angles		dihedrals					
r <sub>eq</sub>	b	θ <sub>eq</sub>	a	IDIVF <sup>a</sup>	V <sub>1</sub> /2	V <sub>2</sub> /2	V <sub>3</sub> /2	V <sub>4</sub> /2	γ
x-x <sup>b</sup>	x-x-ca <sup>b</sup>	ca-x-x-ca <sup>b</sup>							
2.330 (2.743)	109.0 (71.6)	104.53 (100.92)	67.13 (40.47)	1	-1.85 (-1.47)	-1.62 (-2.71)	-0.66 (-0.59)	0.00 (0.02)	180
x-ca <sup>b</sup>	x-ca-ca <sup>b</sup>	x-x-ca-ca <sup>b</sup>							
1.948 (2.145)	143.5 (122.8)	124.14 (119.94)	86.16 (78.24)	1	1.43 (0.90)	-0.19 (-0.20)	-1.11 (-0.69)	0.13 (0.09)	180
ca-ca	ca-ca-ca	x/ca-ca-ca-ca							
1.387	478.4	119.97	67.18	x/ca/ha-ca-ca-ha					
ca-ha	ca-ca-ha	ca/ha-ca-ca-nh							
1.087	344.3	120.01	48.46	4	-	14.5	-	-	180
hn-nh	ca-ca-nh	ca-ca-nh-hn							
1.014	401.2	120.13	69.34	4	-	4.2	-	-	180
ca-nh	hn-nh-hn								
1.364	449.0	114.85	40.05						
		ca-nh-hn							
		116.13	49.08						

**Table S2.** Force–field parameters; values for Te analogue are given in brackets. <sup>a</sup> This is the factor which divides the barriers. <sup>b</sup> New parameters

(p-OCH <sub>3</sub> -PhX) <sub>2</sub>									
bonds		angles		dihedrals					
r <sub>eq</sub>	b	θ <sub>eq</sub>	a	IDIVF <sup>a</sup>	V <sub>1</sub> /2	V <sub>2</sub> /2	V <sub>3</sub> /2	V <sub>4</sub> /2	γ
x-x <sup>b</sup>		x-x-ca <sup>b</sup>		ca-x-x-ca <sup>b</sup>					
2.330 (2.743)	109.0 (71.6)	104.53 (100.92)	67.13 (40.47)	1	-1.85 (-1.47)	-1.62 (-2.71)	-0.66 (-0.59)	0.00 (0.02)	180
x-ca <sup>b</sup>		x-ca-ca <sup>b</sup>		x-x-ca-ca <sup>b</sup>					
1.948 (2.145)	143.5 (122.8)	124.14 (119.94)	86.16 (78.24)	1	-7.70 (1.26)	-0.11 (-0.18)	-1.40 (0.90)	0.21 (0.09)	180
ca-ca		ca-ca-ca		x/ca-ca-ca-ca					
1.387	478.4	119.97	67.18	x/ca/ha-ca-ca-ha					
ca-ha		ca-ca-ha		ca/ha-ca-ca-os					
1.087	344.3	120.01	48.46	4	-	14.5	-	-	180
ca-os		ca-ca-os		ca-ca-os-c3					
1.373	372.4	119.20	69.79	2	-	1.8	-	-	180
c3-os		h1-c3-os		h1-c3-os-ca					
1.439	301.5	108.82	50.84	3	-	-	1.15	-	0
c3-h1		c3-os-ca							
1.093	335.9	117.97	62.27						
		h1-c3-h1							
		109.55	39.18						

**Table S3.** Force–field parameters; values for Te analogue are given in brackets. <sup>a</sup> This is the factor which divides the barriers. <sup>b</sup> New parameters

(p-CH <sub>3</sub> -PhX) <sub>2</sub>									
bonds		angles		dihedrals					
r <sub>eq</sub>	b	θ <sub>eq</sub>	a	IDIVF <sup>a</sup>	V <sub>1</sub> /2	V <sub>2</sub> /2	V <sub>3</sub> /2	V <sub>4</sub> /2	γ
x–x	<sup>b</sup>	x–x–ca	<sup>b</sup>	ca–x–x–ca					
2.330 (2.743)	109.0 (71.6)	104.53 (100.92)	67.13 (40.47)	1	-1.85 (-1.47)	-1.62 (-2.71)	-0.66 (-0.59)	0.00 (0.02)	180
x–ca	<sup>b</sup>	x–ca–ca	<sup>b</sup>	x–x–ca–ca					
1.948 (2.145)	143.5 (122.8)	124.14 (119.94)	86.16 (78.24)	1	-1.25 (1.03)	0.12 (0.02)	-1.43 (-0.71)	0.16 (0.08)	180
ca–ca		ca–ca–ca		ca–ca–c3–hc					
1.387	478.4	119.97	67.18	6	—	—	-2.91	—	180
ca–ha		ca–ca–ha		x/ca/c3–ca–ca–ca					
1.087	344.3	120.01	48.46	x/ca/ha/c3–ca–ca–ha					
c3–ca		ca–c3–hc		4	—	14.5	—	—	180
1.513	323.5	110.15	46.96						
c3–hc		c3–ca–ca							
1.092	337.3	120.63	63.84						
		hc–c3–hc							
		108.35	39.43						

**Table S4.** Force–field parameters; values for Te analogue are given in brackets. <sup>a</sup> This is the factor which divides the barriers. <sup>b</sup> New parameters

(p-Cl-PhX) <sub>2</sub>									
bonds		angles		dihedrals					
r <sub>eq</sub>	b	θ <sub>eq</sub>	a	IDIVF <sup>a</sup>	V <sub>1</sub> /2	V <sub>2</sub> /2	V <sub>3</sub> /2	V <sub>4</sub> /2	γ
x–x	<sup>b</sup>	x–x–ca	<sup>b</sup>	ca–x–x–ca					
2.330 (2.743)	109.0 (71.6)	104.53 (100.92)	67.13 (40.47)	1	-1.85 (-1.47)	-1.62 (-2.71)	-0.66 (-0.59)	0.00 (0.02)	180
x–ca	<sup>b</sup>	x–ca–ca	<sup>b</sup>	x–x–ca–ca					
1.948 (2.145)	143.5 (122.8)	124.14 (119.94)	86.16 (78.24)	1	-0.62 (0.69)	0.17 (0.05)	-1.05 (-0.86)	0.16 (0.10)	180
ca–ca		ca–ca–ca		x/ca–ca–ca–ca					
1.387	478.4	119.97	67.18	x/ca/ha–ca–ca–ha					
ca–ha		ca–ca–ha		ca–ca–ca–cl					
1.087	344.3	120.01	48.46	4	—	14.5	—	—	180
ca–cl		ca–ca–cl							
1.729	322.8	119.4	58.52						

**Table S5.** Force–field parameters; values for Te analogue are given in brackets. <sup>a</sup> This is the factor which divides the barriers. <sup>b</sup> New parameters

(p-NO <sub>2</sub> -PhX) <sub>2</sub>									
bonds		angles		dihedrals					
r <sub>eq</sub>	b	θ <sub>eq</sub>	a	IDIVF <sup>a</sup>	V <sub>1</sub> /2	V <sub>2</sub> /2	V <sub>3</sub> /2	V <sub>4</sub> /2	γ
x–x <sup>b</sup>		x–x–ca <sup>b</sup>		ca–x–x–ca <sup>b</sup>					
2.330 (2.743)	109.0 (71.6)	104.53 (100.92)	67.13 (40.47)	1	-1.85 (-1.47)	-1.62 (-2.71)	-0.66 (-0.59)	0.00 (0.02)	180
x–ca <sup>b</sup>		x–ca–ca <sup>b</sup>		x–x–ca–ca <sup>b</sup>					
1.948 (2.145)	143.5 (122.8)	124.14 (119.94)	86.16 (78.24)	1	11.96 (-1.21)	0.39 (0.40)	-0.33 (1.69)	0.02 (0.00)	180
ca–ca		ca–ca–ca		x/ca–ca–ca–ca					
1.387	478.4	119.97	67.18	x/ca/ha–ca–ca–ha					
ca–ha		ca–ca–ha		ca/ha–ca–ca–no					
1.087	344.3	120.01	48.46	4	–	14.5	–	–	180
no–o		ca–ca–no		ca–ca–no–o					
1.219	761.2	119.54	66.88	4	–	2.4	–	–	180
ca–no		o–no–o							
1.468	322.6	125.13	77.15						
		ca–no–o							
		118.1							
		68.74							

**Table S6.** Relevant interatomic distances ( $\text{\AA}$ ) and angles ( $^\circ$ ) of the fully optimized dichalcogenides; level of theory: B3LYP/6-311G(d,p),SDD. When available, parameters from the crystallographic structures taken from CSD are given in brackets.

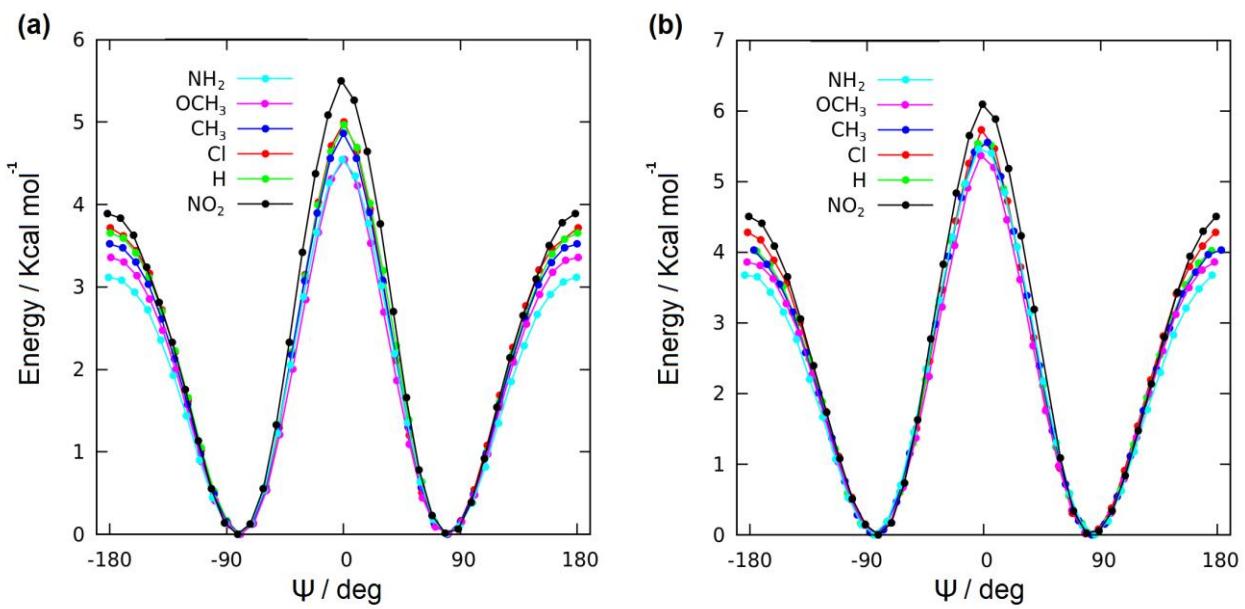
	CSD identifier	X–X'	C <sub>x</sub> –X C <sub>x'</sub> –X'	C <sub>x</sub> –X–X' C <sub>x'</sub> –X'–X	C <sub>x</sub> –X–X'–C <sub>x'</sub> ( $\Psi$ )	C <sub>1</sub> –C <sub>x</sub> –X–X' C <sub>1'</sub> –C <sub>x'</sub> –X'–X ( $\Phi_{1,2}$ )
(p-NH <sub>2</sub> -PhSe) <sub>2</sub>	—	2.52	1.94 1.94	103 103	-81	94 94
(p-NH <sub>2</sub> -PhTe) <sub>2</sub>	—	2.86	2.12 2.12	101 101	-84	92 92
(p-CH <sub>3</sub> O-PhSe) <sub>2</sub>	—	2.51	1.94 1.94	102 102	-79	93 95
(p-CH <sub>3</sub> O-PhTe) <sub>2</sub>	BAJHAV	2.85 (2.715)	2.13 (2.139) 2.13 (2.143)	101 (99.8) 101 (100.3)	-82 (-81)	93 (12) 93 (20)
(p-CH <sub>3</sub> -PhSe) <sub>2</sub>	QQQGBV01	2.50 (2.328)	1.95 (1.923) 1.95 (1.910)	102 (102.0) 102 (101.2)	80 (100)	87 (90) -96 (-73)
(p-CH <sub>3</sub> -PhTe) <sub>2</sub>	DPTOTE	2.84 (2.696)	2.13 (2.125) 2.13 (2.131)	100 (101.5) 100 (100.0)	83 (86)	90 (37) 90 (37)
(PhSe) <sub>2</sub>	YUXPIR	2.50 (2.307)	1.95 (1.946) 1.95 (1.934)	101 (102.4) 101 (103.5)	80 (85)	-96 (-23) 87 (0)
(PhTe) <sub>2</sub>	DPHDTE01	2.84 (2.707)	2.14 (2.131) 2.14 (2.115)	100 (100.7) 100 (97.7)	-85 (-90)	-90 (-84) 92 (90)
(p-Cl-PhSe) <sub>2</sub>	CLPHSE	2.50 (2.332)	1.95 (1.929) 1.95 (1.911)	101 (98.6) 101 (98.9)	-79 (-74)	-85 (-61) 98 (74)
(p-Cl-PhTe) <sub>2</sub>	CLPHTE01	2.84 (2.680)	2.14 (2.144) 2.14 (2.160)	100 (99.6) 100 (101.6)	-82 (-89)	-88 (-13) -88 (-10)
(p-NO <sub>2</sub> -PhSe) <sub>2</sub>	DUWKEL	2.49 (2.302)	1.96 (1.921) 1.96 (1.921)	101 (103.2) 101 (103.2)	-82 (-88)	103 (23) 103 (23)
(p-NO <sub>2</sub> -PhTe) <sub>2</sub>	—	2.834	2.140 2.140	99.2 99.2	-82	98 98

**Table S7.** Molecular dipole moments in Debye calculated with *ab initio* density and dipole integrals using the B3LYP/cc-pVTZ(-PP) *open/closed* geometry (A) and from RESP charges using the MM equilibrium geometry (B). Values for the Te compounds are given in parentheses.

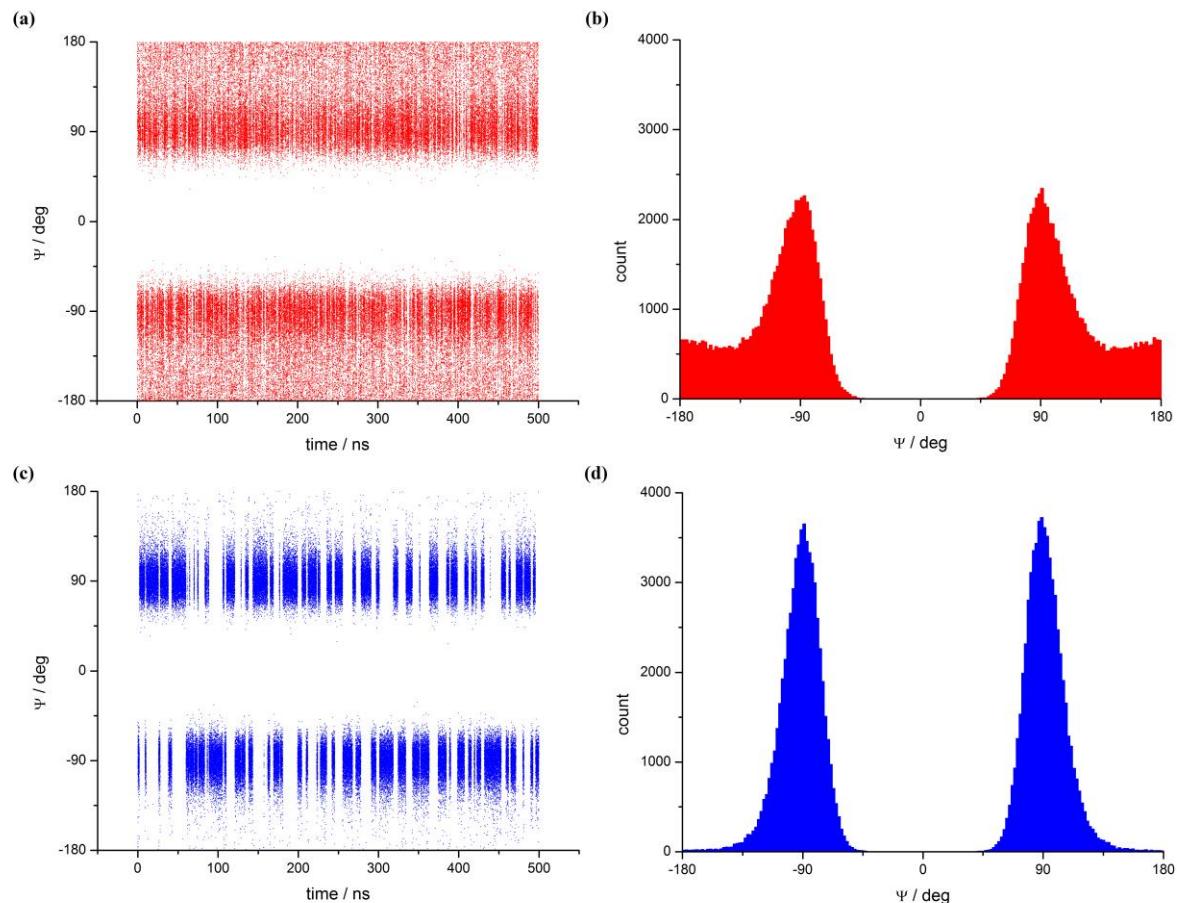
	(p-NH <sub>2</sub> -PhX) <sub>2</sub>	(p-OCH <sub>3</sub> -PhX) <sub>2</sub>	(p-CH <sub>3</sub> -PhX) <sub>2</sub>	(PhX) <sub>2</sub>	(p-Cl-PhX) <sub>2</sub>	(p-NO <sub>2</sub> -PhX) <sub>2</sub>	
A	open	5.22 (4.80)	1.74 (1.11)	3.35 (2.95)	2.81 (2.39)	0.32 (0.46)	4.59 (5.21)
	closed	4.26 (2.34)	1.76 (1.40)	2.66 (2.49)	2.11 (1.86)	0.90 (1.10)	5.10 (5.73)
B	MM	4.55 (3.00)	1.35 (1.51)	3.11 (2.82)	2.54 (2.29)	0.60 (0.84)	5.02 (5.70)

**Table S8.**  $\sigma_{GAFF}$  values vs vdW radii for C, N, O, P, S, F, Cl, Br, I atoms; values for Se and Te are extrapolated and are those used in the work. For GAFF parameters O is the TIP3P water oxygen.

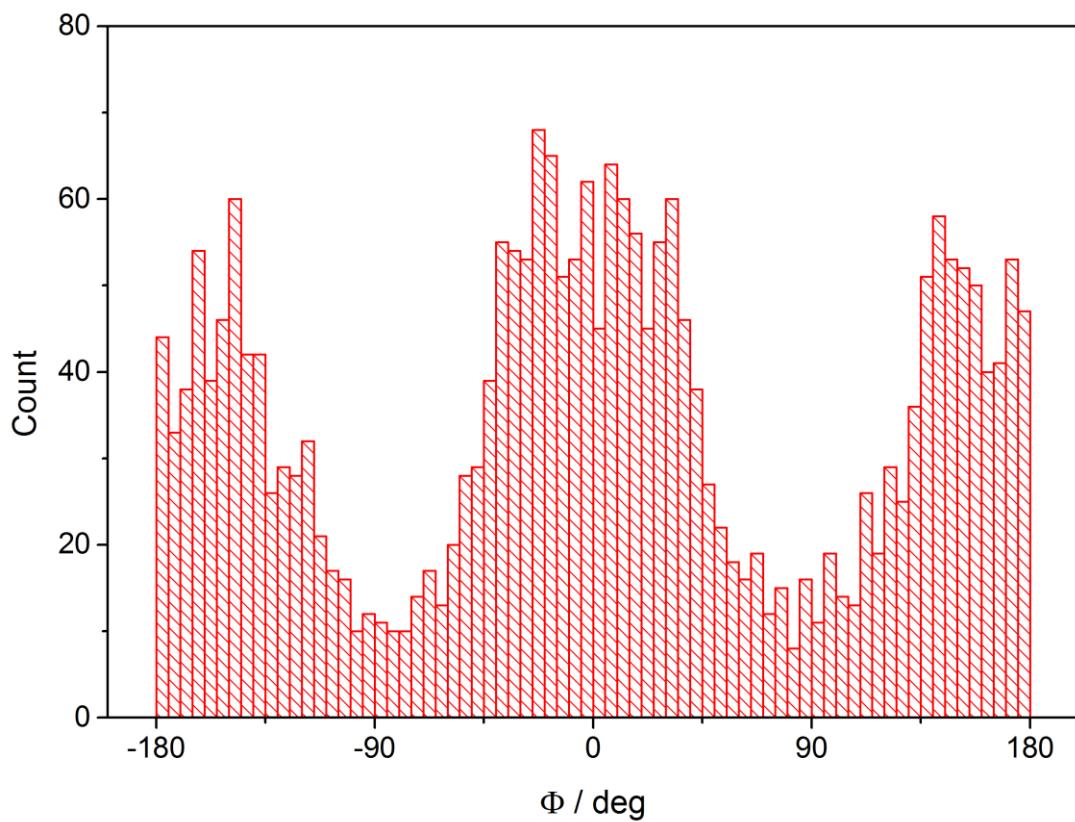
Atom	VDW radius / Å	$\sigma_{GAFF}$ / Å
C	1.70	1.90
N	1.55	1.82
O <sup>a</sup>	1.52	1.76
F	1.47	1.75
P	1.80	2.10
S	1.80	2.00
Cl	1.75	1.948
Se	1.90	2.12
Br	1.85	2.02
Te	2.06	2.26
I	1.98	2.15



**Figure S1.** Energy profiles at B3LYP/6-311G(d,p),SDD level of theory for the rotation of  $\Psi$  of all Se (a) and Te (b) diphenyl compounds.



**Figure S2.** Trajectories a (c) and distributions b (d) in chloroform of (PhSe)<sub>2</sub> (red) and (PhTe)<sub>2</sub> (blue).



**Figure S3.** Distributions (1250 structures) in chloroform of  $(\text{PhSe})_2$