SUPPLEMENTARY INFORMATION

System	(3,-3) L(**r**) CP type [a]	R(N), a.u.[b]	R(O), a.u.[b]	R(C), a.u.[b]	L($\mathbf{r}_{CP}$), a.u.	$\rho(\mathbf{r}_{CP})$, a.u.
PZDO init.	**N**-C b.m.	0.785	-	1.773	2.497	0.540
	N-C b.m.	0.785	-	1.773	2.497	0.540
	N-O b.m.	0.800	1.624	-	2.149	0.513
PZDO cryst init.	**N**-C b.m.	0.786	-	1.802	2.427	0.531
	N-C b.m.	0.786	-	1.803	2.425	0.531
	N-O b.m.	0.800	1.655	-	2.092	0.504
PZDO DR	**N**-C b.m.	0.805	-	1.873	1.961	0.482
	N-C b.m.	0.805	-	1.873	1.961	0.482
	N-O b.m.	0.836	1.874	-	1.199	0.399
	LP	0.743	2.966	3.000, 3.000	2.738	0.573
PZDO cryst. DR	**N**-C b.m.	0.805	-	1.864	1.974	0.484
	N-C b.m.	0.804	-	1.866	1.973	0.484
	N-O b.m.	0.835	1.981	-	1.075	0.383
	LP	0.743	3.053	2.990, 2.996	2.717	0.571
TeMePzDO init.	**N**-C b.m.	0.786	-	1.789	2.428	0.534
	N-C b.m.	0.786	-	1.789	2.428	0.534
	N-O b.m.	0.804	1.632	-	2.062	0.505
TeMePzDO cryst init.	**N**-C b.m.	0.787	-	1.824	2.349	0.525
	N-C b.m.	0.787	-	1.824	2.350	0.524
	N-O b.m.	0.804	1.651	-	2.024	0.498
TeMePzDO DR	**N**-C b.m.	0.804	-	1.896	1.949	0.480
	N-C b.m.	0.804	-	1.896	1.949	0.480
	N-O b.m.	0.838	1.881	-	1.151	0.394
	LP	0.742	2.974	3.018, 3.018	2.771	0.576
TeMePzDO cryst DR	**N**-C b.m.	0.804	-	1.880	1.965	0.482
	N-C b.m.	0.804	-	1.881	1.957	0.482
	N-O b.m.	0.836	1.976	-	1.073	0.383
	LP	0.744	3.039	2.991, 3.001	2.721	0.571

Table SI1: Bonded ("b.m.") and lone pair ("LP") (3,-3) critical point (CP) maxima of the $L(\mathbf{r}) = -\nabla^2(\mathbf{r})$ distribution in the valence-shell charge concentration (VSCC) of the N atom for both the systems generated in the case of molecular SMD treatment (*i.e.* calculated thanks to the Gaussian package) and the molecular complexes which are present in intercalated crystalline PZDO/TeMePzDO most stable relaxed phases (*i.e.* obtained through VASP calculations).

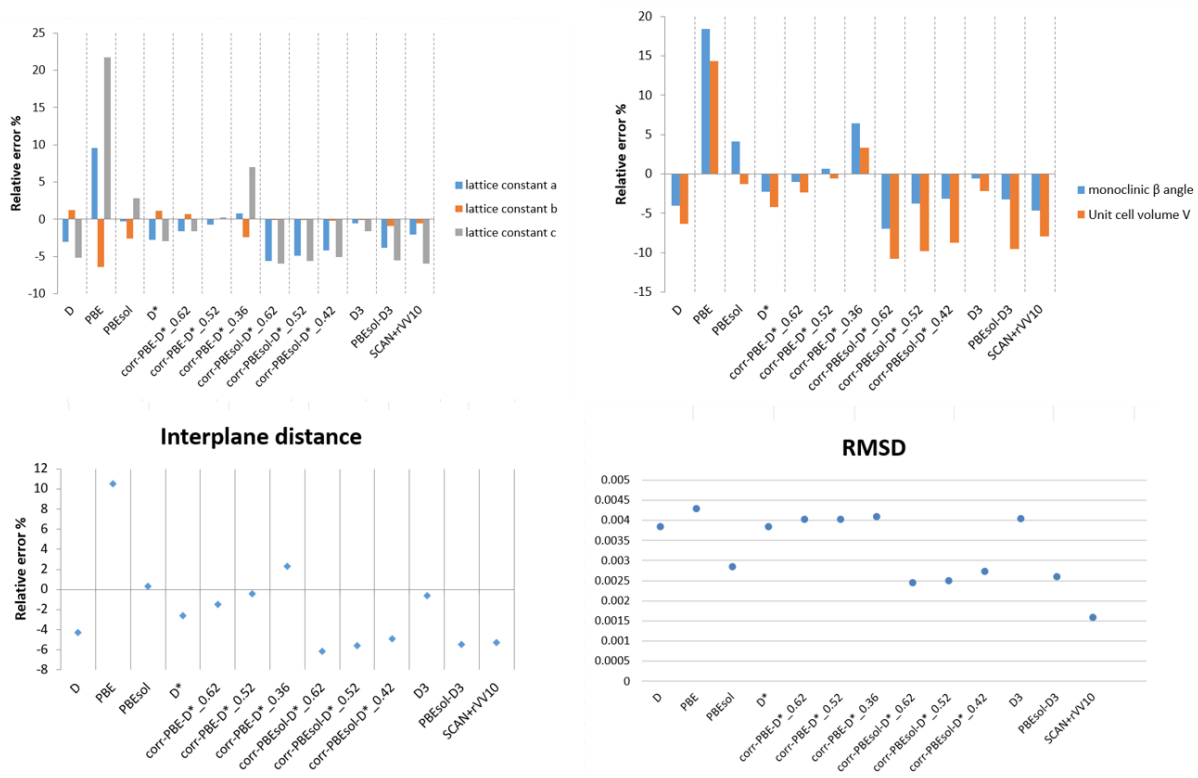


Figure SI1: Relative errors (%) of DFT calculated values to experiment for the PZDO crystal: (a) for the optimized lattice parameters: *a*, *b* and *c*, and (b)
for the unit-cell volume V and the monoclinic angle β; c) Relative errors (%) of DFT calculated values to experiment for the inter-plane distance, *d*. d) RMSD values with respect to experimental data for the intramolecular bond lengths and intermolecular distances without taking into account covalent bonds involving either H atoms or H-bonding interactions.

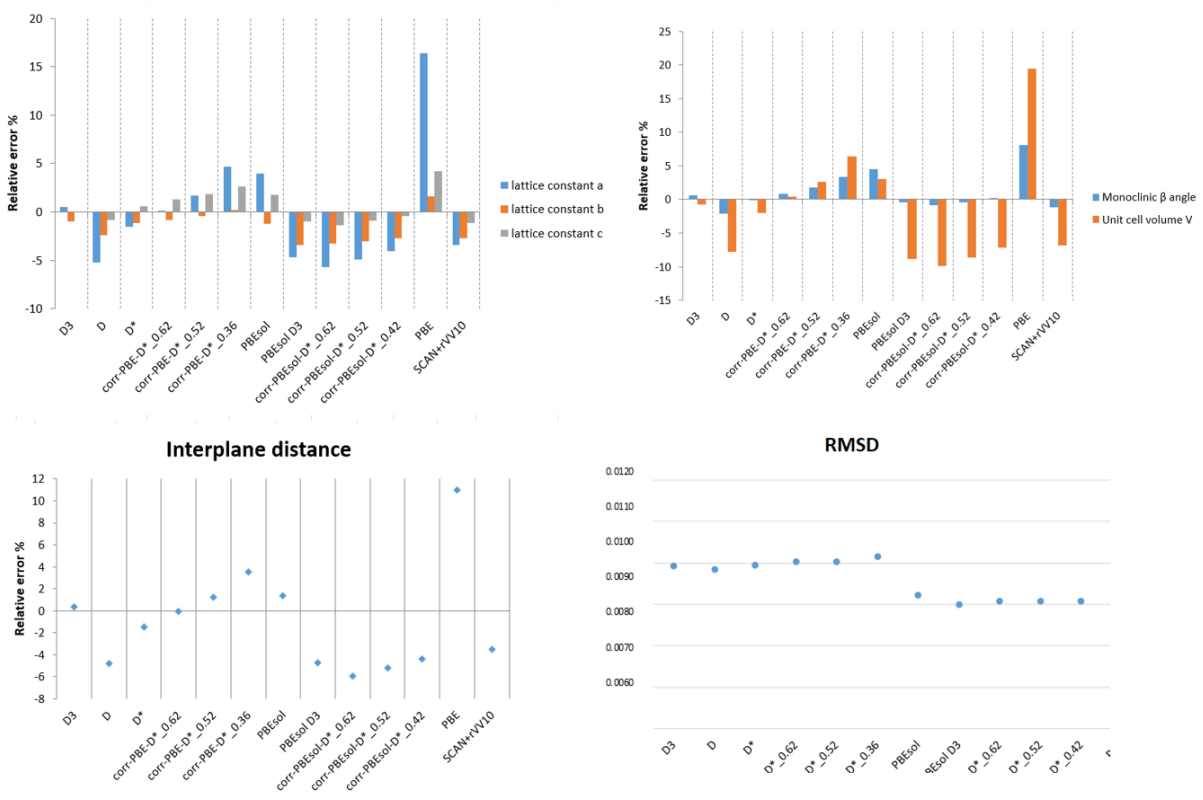
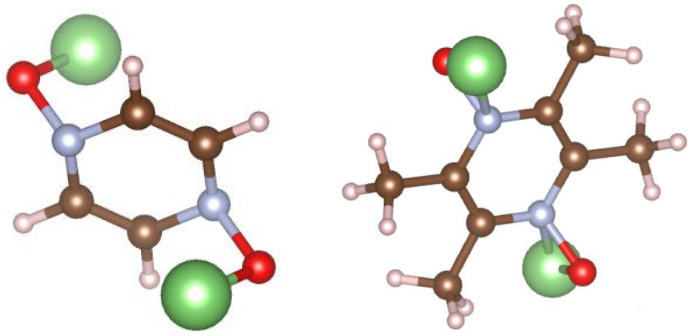


Figure SI2: Relative errors (%) of DFT calculated values to experiment for the TeMePzDO crystal: (a) for the optimized lattice parameters: *a*, *b* and *c*, and (b) for the unit-cell volume V and the monoclinic angle β; c) Relative errors (%) of DFT calculated values to experiment for the inter-plane distance, *d*. d) RMSD values with respect to experimental data for the intramolecular bond lengths and intermolecular distances without taking into account covalent bonds involving either H atoms or H-bonding interactions.



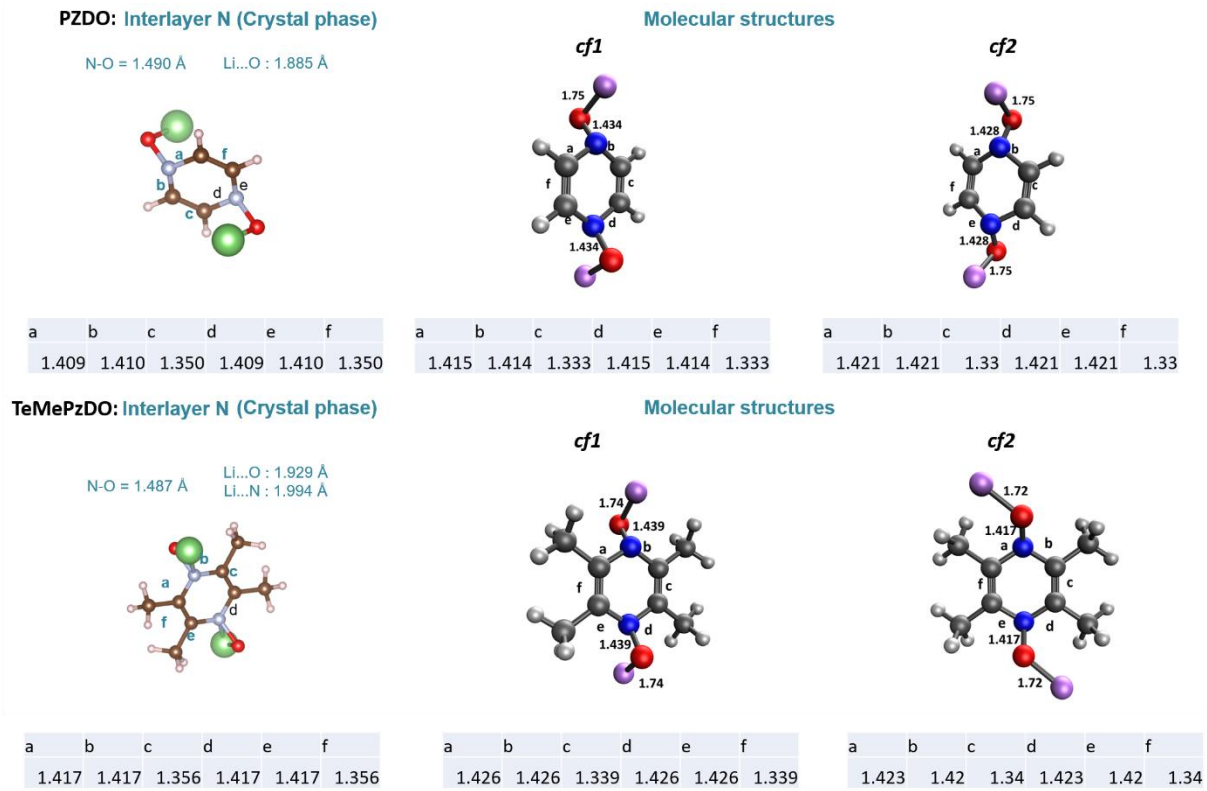


Figure SI3: Top: relaxed molecular structure extracted from the most stable intercalated PZDO and TeMePzDO crystalline phases; middle and bottom: comparison of their bond length (left) with those of molecular complexes (middle and right corresponding to two distinct conformations, *cf1* and *cf2*).

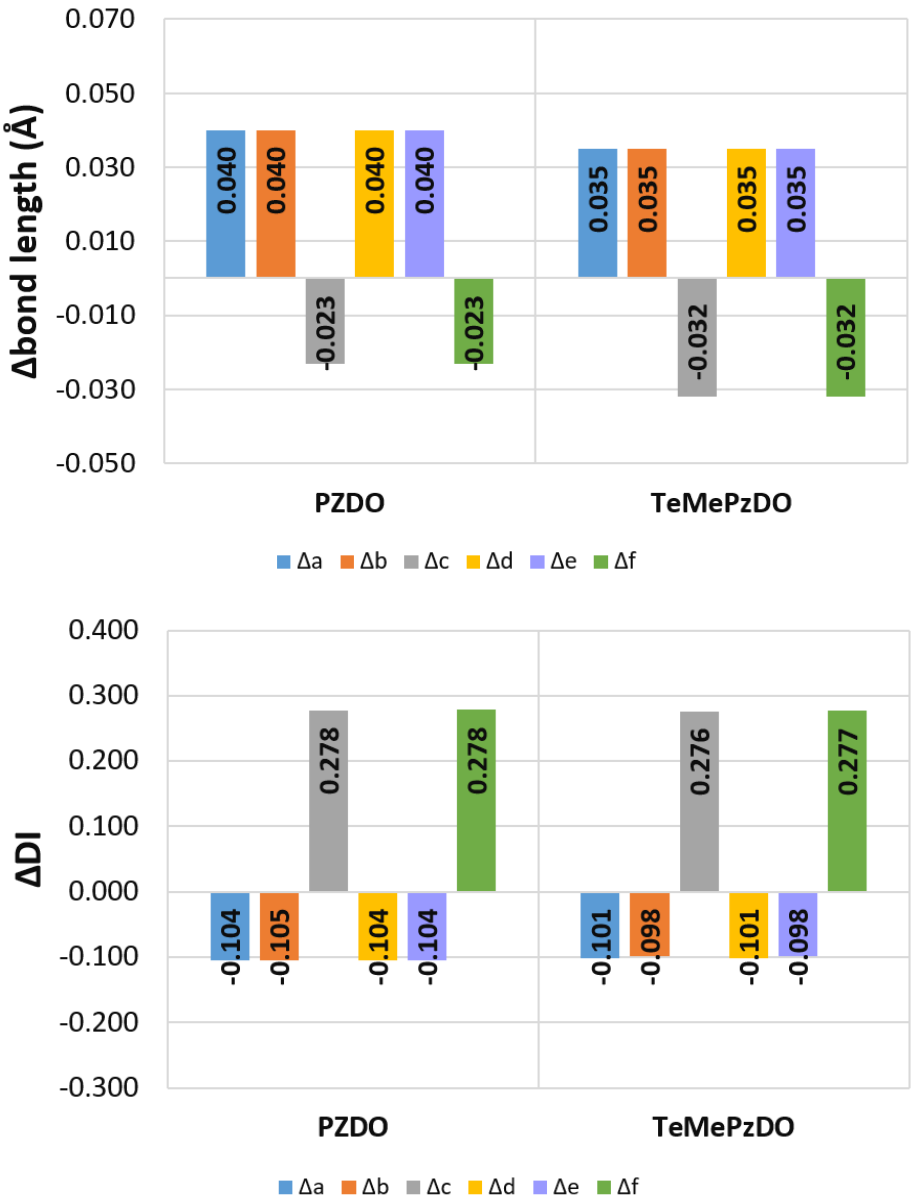


Figure SI4: Top: Calculated bond length variations (Δbond length) of each bond in the ring for the single (left) and double (right) reduction process characterizing molecular species in the intercalated crystalline structures; bottom: calculated DI variations (ΔDI) of each bond in the ring for the single (left) and double (right) reduction process in the intercalated crystalline structures.

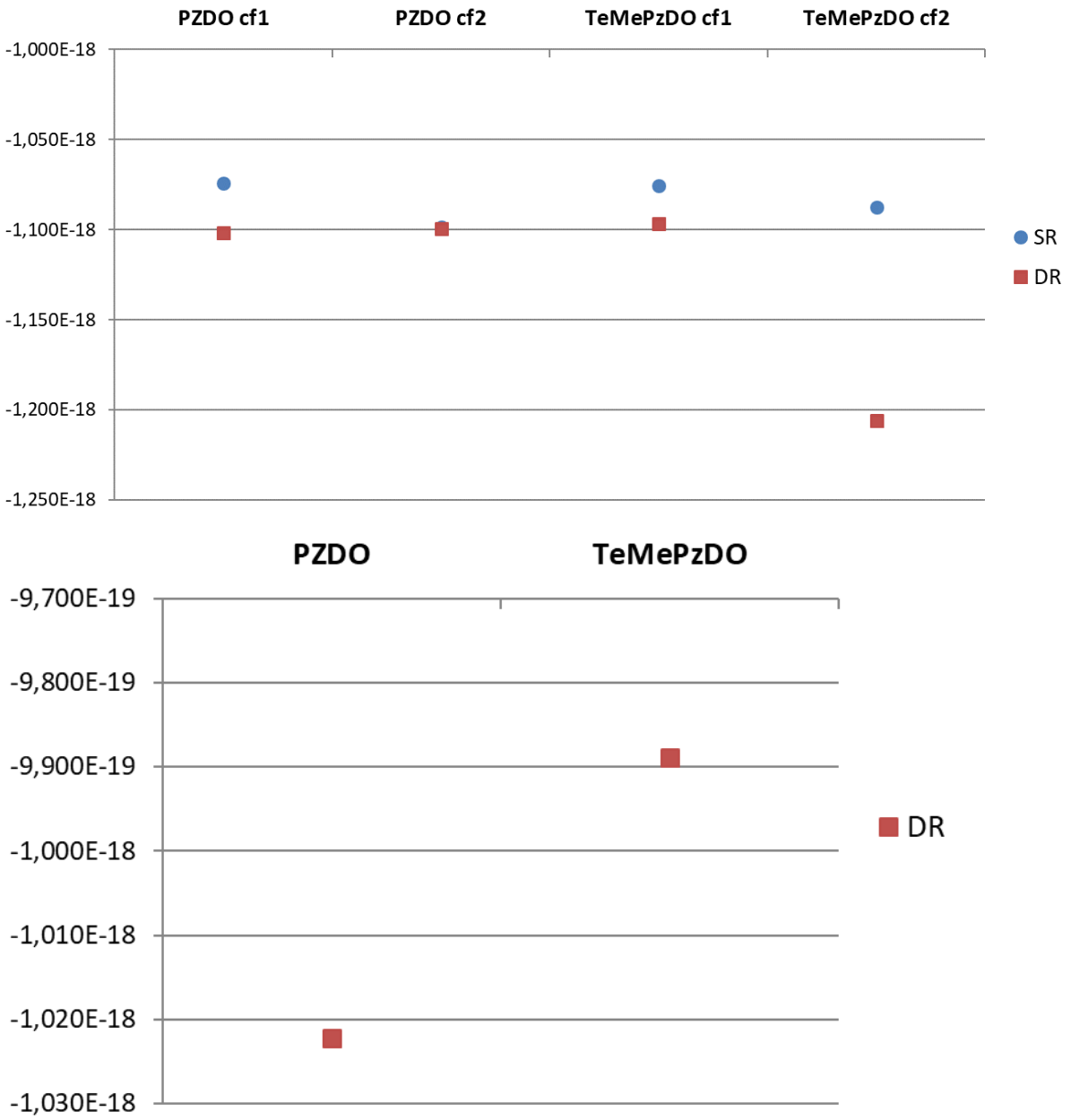
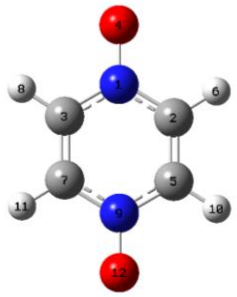


Figure SI5: (a) Estimation of the electrostatic interactions energy (in Joule), between the Li^+ cations and the oxygen atoms: top: in the case of molecular species; bottom: for the same complexes, which are present in the intercalated crystal phases.

Part 2. Calculated Structures of PZDO and TeMePzDO (molecular) and under Single and Double reduced forms with Li calculated at the M062X/6-311+G(2d,2p) with implicit SMD solvent (acetonitrile) model

The structural parameters (bond lengths, bond/dihedral angles) – all defined with respect to the initial molecular Z-matrix of each compound (*i.e.* either PZDO or TeMePzDO) – are displayed in the following Tables for the three kinds of states (initial, singly reduced, doubly reduced) considered in this investigation.

2-1) PZDO (D_{2h}-symmetry) Z-Matrix along with corresponding structural parameters

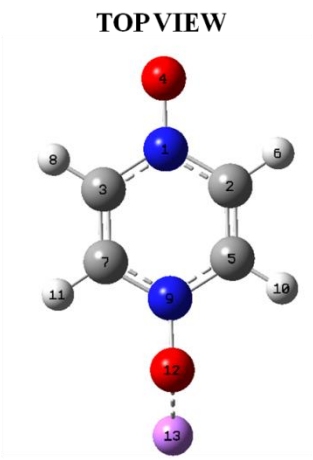


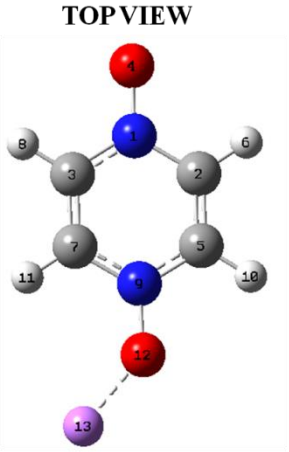
N						
C	1	B1				
C	1	B2	2	A1		
O	1	B3	2	A2	3	D1
C	2	B4	1	A3	4	D2
H	2	B5	1	A4	4	D3
C	3	B6	1	A5	4	D4
H	3	B7	1	A6	4	D5
N	7	B8	3	A7	1	D6
H	5	B9	2	A8	1	D7
H	7	B10	3	A9	1	D8
O	9	B11	7	A10	3	D9

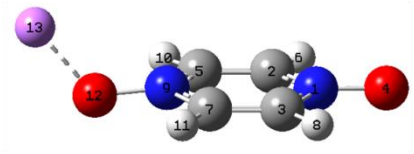
Bond lengths (Å)		Bond angles (degree)		Dihedral angles (degree)	
B1	1.3534				
B2	1.3534	**A1**	117.66		
B3	1.2825	**A2**	121.17	**D1**	180.
B4	1.3677	**A3**	121.17	**D2**	180.
B5	1.0775	**A4**	116.21	**D3**	0.
B6	1.3677	**A5**	121.17	**D4**	180.
B7	1.0775	**A6**	116.21	**D5**	0.
B8	1.3534	**A7**	121.17	**D6**	0.
B9	1.0775	**A8**	122.62	**D7**	180.
B10	1.0775	**A9**	122.62	**D8**	180.
B11	1.2825	**A10**	121.17	**D9**	180.

Table SI-2: Calculated structural parameters for the molecular (unreduced) PZDO system.

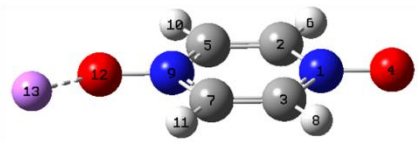
2-2) Singly Reduced (SR) Li-(*cf1*)-PZDO and Li-(*cf2*)-PZDO Z-Matrices along with corresponding structural parameters







$\delta(Li\text{-}O_{12}\text{-}N_9\text{-}C_7) = 95.9$
$\delta(O_{12}\text{-}N_9\text{-}C_7\text{-}C_3) = 172.8$
(*cf1*)



$\delta(Li\text{-}O_{12}\text{-}N_9\text{-}C_7) = 13.0$
$\delta(O_{12}\text{-}N_9\text{-}C_7\text{-}C_3) = 178.8$
(*cf2*)

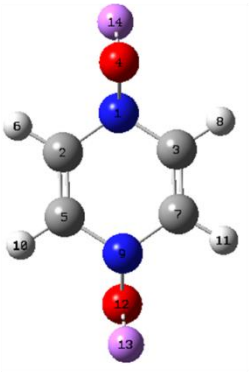
N						
C	1	B1				
C	1	B2	2	A1		
O	1	B3	2	A2	3	D1
C	2	B4	1	A3	4	D2
H	2	B5	1	A4	4	D3
C	3	B6	1	A5	4	D4
H	3	B7	1	A6	4	D5
N	7	B8	3	A7	1	D6
H	5	B9	2	A8	1	D7
H	7	B10	3	A9	1	D8
O	9	B11	7	A10	3	D9
Li	12	B12	9	A11	7	D10

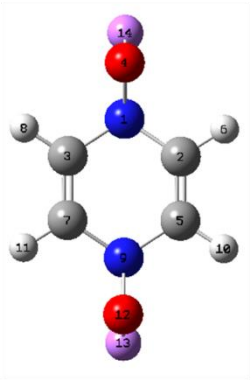
Li-(*cf1*)-PZDO						Li-(*cf2*)-PZDO					
Bond-lengths (Å)		**Bond angles (degree)**		**Dihedral angles (degree)**		**Bond lengths (Å)**		**Bond angles (degree)**		**Dihedral angles (degree)**	
B1	1.3814					**B1**	1.3820				
B2	1.3814	**A1**	117.26			**B2**	1.3801	**A1**	117.27		
B3	1.3160	**A2**	121.36	**D1**	178.0	**B3**	1.3169	**A2**	121.34	**D1**	179.6
B4	1.3521	**A3**	121.27	**D2**	-179.3	**B4**	1.3520	**A3**	121.30	**D2**	-179.8
B5	1.0774	**A4**	116.04	**D3**	0.5	**B5**	1.0773	**A4**	116.06	**D3**	0.1
B6	1.3521	**A5**	121.27	**D4**	179.3	**B6**	1.3524	**A5**	121.33	**D4**	179.8
B7	1.0774	**A6**	116.04	**D5**	-0.5	**B7**	1.0774	**A6**	116.08	**D5**	-0.1
B8	1.3732	**A7**	120.95	**D6**	-0.8	**B8**	1.3733	**A7**	120.89	**D6**	-0.1
B9	1.0778	**A8**	122.63	**D7**	-179.8	**B9**	1.0777	**A8**	122.72	**D7**	-180.0
B10	1.0778	**A9**	122.63	**D8**	179.8	**B10**	1.0782	**A9**	122.34	**D8**	179.9
B11	1.3522	**A10**	120.44	**D9**	172.8	**B11**	1.3428	**A10**	121.70	**D9**	178.8
B12	1.7505	**A11**	124.77	**D10**	95.9	**B12**	1.7284	**A11**	137.39	**D10**	13.0

Table SI-3: Calculated structural parameters for Singly Reduced (SR) Li-PZDO systems.

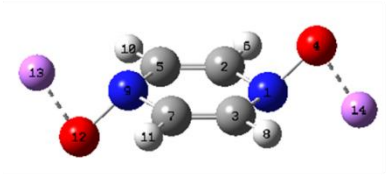
2-3) 2Li-(*cf1*)-PZDO and 2Li-(*cf2*)-PZDO Z-Matrices along with corresponding structural parameters

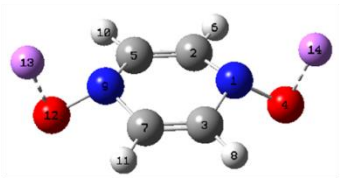
TOP VIEW **TOP VIEW**





SIDE VIEW **SIDE VIEW**





$\delta(Li\text{-}O_{12}\text{-}N_9\text{-}C_7)= 116.9$ $\delta(Li\text{-}O_4\text{-}N_1\text{-}C_2)= -116.9$
$\delta(O_{12}\text{-}N_9\text{-}C_7\text{-}C_3)= 127.7$ $\delta(O_4\text{-}N_1\text{-}C_2\text{-}C_5)= -127.7$

(*cf1*)

$\delta(Li\text{-}O_{12}\text{-}N_9\text{-}C_7)= 117.6$ $\delta(Li\text{-}O_4\text{-}N_1\text{-}C_2)= 117.6$
$\delta(O_{12}\text{-}N_9\text{-}C_7\text{-}C_3)= 143.0$ $\delta(O_4\text{-}N_1\text{-}C_2\text{-}C_5)= 143.0$

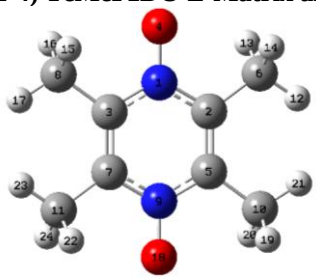
(*cf2*)

N						
C	1	B1				
C	1	B2	2	A1		
O	1	B3	2	A2	3	D1
C	2	B4	1	A3	4	D2
H	2	B5	1	A4	4	D3
C	3	B6	1	A5	4	D4
H	3	B7	1	A6	4	D5
N	7	B8	3	A7	1	D6
H	5	B9	2	A8	1	D7
H	7	B10	3	A9	1	D8
O	9	B11	7	A10	3	D9
Li	12	B12	9	A11	5	D10
Li	4	B13	1	A12	2	D11

2Li-(*cf1*)-PZDO						**2Li-(*cf2*)-PZDO**					
Bond-lengths (Å)		**Bond angles (degree)**		**Dihedral angles (degree)**		**Bond lengths (Å)**		**Bond angles (degree)**		**Dihedral angles (degree)**	
B1	1.4145					**B1**	1.4208				
B2	1.4145	**A1**	112.44			**B2**	1.4208	**A1**	111.27		
B3	1.4337	**A2**	111.26	**D1**	-125.5	**B3**	1.4282	**A2**	111.33	**D1**	124.8
B4	1.3333	**A3**	123.76	**D2**	-127.7	**B4**	1.3301	**A3**	123.03	**D2**	143.0
B5	1.0803	**A4**	114.89	**D3**	51.8	**B5**	1.0790	**A4**	114.76	**D3**	-39.7
B6	1.3333	**A5**	123.76	**D4**	127.7	**B6**	1.3301	**A5**	123.01	**D4**	-143.0
B7	1.0803	**A6**	114.90	**D5**	-51.8	**B7**	1.0790	**A6**	114.77	**D5**	39.7
B8	1.4145	**A7**	123.76	**D6**	-2.4	**B8**	1.4208	**A7**	123.03	**D6**	0.0
B9	1.0803	**A8**	121.34	**D7**	-177.0	**B9**	1.0790	**A8**	122.16	**D7**	177.2
B10	1.0803	**A9**	121.35	**D8**	177.1	**B10**	1.0790	**A9**	122.16	**D8**	-177.2
B11	1.4337	**A10**	111.26	**D9**	127.7	**B11**	1.4282	**A10**	111.33	**D9**	143.0
B12	1.7497	**A11**	75.19	**D10**	116.9	**B12**	1.7493	**A11**	75.41	**D10**	117.6
B13	1.7497	**A12**	75.19	**D11**	-116.9	**B13**	1.7493	**A12**	75.41	**D11**	117.6

Table SI-4: Calculated structural parameters for the Doubly Reduced (DR) 2Li-PZDO systems.

2-4) TeMePzDO Z-Matrix along with corresponding structural parameters



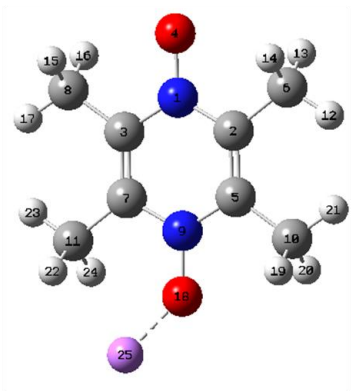
N
C 1 B1
C 1 B2 2 A1
O 1 B3 2 A2 3 D1
C 2 B4 1 A3 4 D2
C 2 B5 1 A4 4 D3
C 3 B6 1 A5 4 D4
C 3 B7 1 A6 4 D5
N 7 B8 3 A7 1 D6
C 5 B9 2 A8 1 D7
C 7 B10 3 A9 1 D8
H 6 B11 2 A10 1 D9
H 6 B12 2 A11 1 D10
H 6 B13 2 A12 1 D11
H 8 B14 3 A13 1 D12
H 8 B15 3 A14 1 D13
H 8 B16 3 A15 1 D14
O 9 B17 7 A16 3 D15
H 10 B18 5 A17 2 D16
H 10 B19 5 A18 2 D17
H 10 B20 5 A19 2 D18
H 11 B21 7 A20 3 D19
H 11 B22 7 A21 3 D20
H 11 B23 7 A22 3 D21

Bond lengths (Å)		Bond angles (degree)		Dihedral angles (degree)	
B1	1.3625				
B2	1.3625	**A1**	121.11		
B3	1.2887	**A2**	119.45	**D1**	-179.9
B4	1.3821	**A3**	119.42	**D2**	179.4
B5	1.4886	**A4**	115.02	**D3**	-0.8
B6	1.3821	**A5**	119.46	**D4**	-179.4
B7	1.4883	**A6**	115.01	**D5**	0.7
B8	1.3625	**A7**	119.42	**D6**	-0.7
B9	1.4883	**A8**	125.53	**D7**	-179.2
B10	1.4886	**A9**	125.56	**D8**	179.1
B11	1.0825	**A10**	111.96	**D9**	-176.9
B12	1.0899	**A11**	109.30	**D10**	-55.5
B13	1.0904	**A12**	109.73	**D11**	61.3
B14	1.0905	**A13**	109.73	**D12**	-61.9
B15	1.0898	**A14**	109.32	**D13**	54.9
B16	1.0824	**A15**	111.92	**D14**	176.3
B17	1.2887	**A16**	119.45	**D15**	-179.4
B18	1.0898	**A17**	109.32	**D16**	124.9
B19	1.0905	**A18**	109.73	**D17**	-118.2
B20	1.0824	**A19**	111.92	**D18**	3.5
B21	1.0899	**A20**	109.30	**D19**	-124.3
B22	1.0825	**A21**	111.96	**D20**	-2.9
B23	1.0904	**A22**	109.73	**D21**	118.9

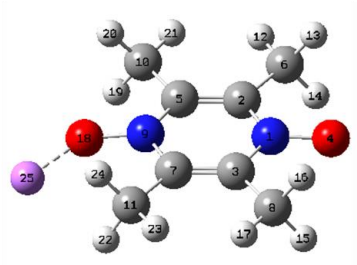
Table SI-5: Calculated structural parameters for the molecular (unreduced) TeMePzDO system.

2-5) Li-(*cf1*)- and Li-(*cf2*)-TeMePzDO Z-Matrices along with corresponding structural parameters

TOP VIEW

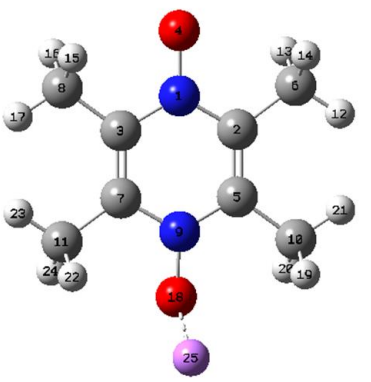


SIDE VIEW

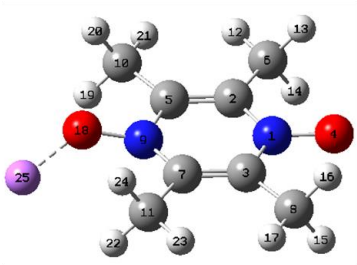


$\delta(\text{Li-O}_{12}\text{-N}_9\text{-C}_5) = 115.7$
$\delta(\text{O}_{12}\text{-N}_9\text{-C}_5\text{-C}_2) = -126.2$
(*cf1*)

TOP VIEW



SIDE VIEW



$\delta(\text{Li-O}_{12}\text{-N}_9\text{-C}_5) = -47.8$
$\delta(\text{O}_{12}\text{-N}_9\text{-C}_5\text{-C}_2) = +133.6$
(*cf2*)

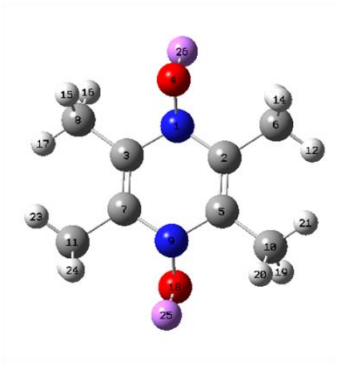
N						
C	1	B1				
C	1	B2	2	A1		
O	1	B3	2	A2	3	D1
C	2	B4	1	A3	4	D2
C	2	B5	1	A4	4	D3
C	3	B6	1	A5	4	D4
C	3	B7	1	A6	4	D5
N	7	B8	3	A7	1	D6
C	5	B9	2	A8	1	D7
C	7	B10	3	A9	1	D8
H	6	B11	2	A10	1	D9
H	6	B12	2	A11	1	D10
H	6	B13	2	A12	1	D11
H	8	B14	3	A13	1	D12
H	8	B15	3	A14	1	D13
H	8	B16	3	A15	1	D14
O	9	B17	7	A16	3	D15
H	10	B18	5	A17	2	D16
H	10	B19	5	A18	2	D17
H	10	B20	5	A19	2	D18
H	11	B21	7	A20	3	D19
H	11	B22	7	A21	3	D20
H	11	B23	7	A22	3	D21
Li	18	B24	9	A23	5	D22

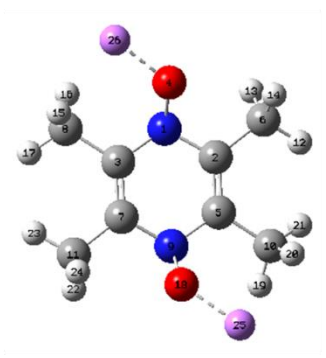
Li-(*cf1*)-TeMePzDO						Li-(*cf2*)-TeMePzDO					
Bond-lengths (Å)		**Bond angles (degree)**		**Dihedral angles (degree)**		**Bond lengths (Å)**		**Bond angles (degree)**		**Dihedral angles (degree)**	
B1	1.3937					**B1**	1.3916				
B2	1.3900	**A1**	120.34			**B2**	1.3916	**A1**	120.30		
B3	1.3218	**A2**	119.79	**D1**	178.7	**B3**	1.3196	**A2**	119.81	**D1**	-176.9
B4	1.3616	**A3**	119.86	**D2**	178.6	**B4**	1.3618	**A3**	119.80	**D2**	-179.2
B5	1.4930	**A4**	114.38	**D3**	-1.7	**B5**	1.4935	**A4**	114.33	**D3**	1.7
B6	1.3623	**A5**	119.75	**D4**	-178.7	**B6**	1.3618	**A5**	119.80	**D4**	179.2
B7	1.4932	**A6**	114.39	**D5**	1.7	**B7**	1.4935	**A6**	114.33	**D5**	-1.7
B8	1.3872	**A7**	119.58	**D6**	-0.5	**B8**	1.3890	**A7**	119.63	**D6**	1.5
B9	1.4947	**A8**	125.69	**D7**	179.6	**B9**	1.4949	**A8**	125.50	**D7**	-179.3
B10	1.4955	**A9**	125.20	**D8**	-179.3	**B10**	1.4949	**A9**	125.50	**D8**	179.3
B11	1.0838	**A10**	111.87	**D9**	-179.7	**B11**	1.0837	**A10**	111.98	**D9**	179.6
B12	1.0906	**A11**	110.17	**D10**	-58.2	**B12**	1.0901	**A11**	110.04	**D10**	-59.0
B13	1.0902	**A12**	110.06	**D11**	59.0	**B13**	1.0906	**A12**	110.11	**D11**	58.1
B14	1.0902	**A13**	109.93	**D12**	-59.0	**B14**	1.0906	**A13**	110.11	**D12**	-58.1
B15	1.0905	**A14**	110.05	**D13**	58.0	**B15**	1.0901	**A14**	110.04	**D13**	59.0
B16	1.0839	**A15**	112.13	**D14**	179.7	**B16**	1.0837	**A15**	111.98	**D14**	-179.6
B17	1.3500	**A16**	119.93	**D15**	171.3	**B17**	1.3633	**A16**	118.20	**D15**	-165.4
B18	1.0900	**A17**	110.46	**D16**	117.7	**B18**	1.0921	**A17**	110.52	**D16**	123.1
B19	1.0904	**A18**	109.93	**D17**	-124.8	**B19**	1.0894	**A18**	110.08	**D17**	-119.1
B20	1.0837	**A19**	111.75	**D18**	-3.7	**B20**	1.0836	**A19**	111.83	**D18**	2.4
B21	1.0945	**A20**	111.11	**D19**	-114.1	**B21**	1.0921	**A20**	110.08	**D19**	-123.1
B22	1.0832	**A21**	111.85	**D20**	5.2	**B22**	1.0836	**A21**	111.83	**D20**	-2.4
B23	1.0942	**A22**	110.44	**D21**	124.4	**B23**	1.0894	**A22**	110.52	**D21**	119.1
B24	1.7258	**A23**	132.67	**D22**	177.3	**B24**	1.7482	**A23**	119.41	**D22**	99.8

Table SI-6: Calculated structural parameters for the Singly Reduced (SR) 1Li-TeMePzDO systems.

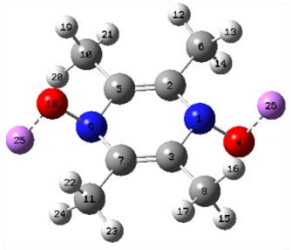
2-6) 2Li-(*cf1*)- and 2Li-(*cf2*)-TeMePzDO Z-Matrices along with corresponding structural parameters

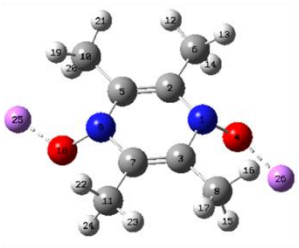
TOP VIEW **TOP VIEW**





SIDE VIEW **SIDE VIEW**





$\delta(Li\text{-}O_{18}\text{-}N_9\text{-}C_5) = 115.7$ $\delta(Li\text{-}O_4\text{-}N_1\text{-}C_2) = -115.7$
$\delta(O_{18}\text{-}N_9\text{-}C_5\text{-}C_2) = -126.2$ $\delta(O_4\text{-}N_1\text{-}C_3\text{-}C_7) = 126.2$

(*cf1*)

$\delta(Li\text{-}O_{18}\text{-}N_9\text{-}C_5) = -47.7$ $\delta(Li\text{-}O_4\text{-}N_1\text{-}C_2) = -47.8$
$\delta(O_{18}\text{-}N_9\text{-}C_5\text{-}C_2) = -132.2$ $\delta(O_4\text{-}N_1\text{-}C_3\text{-}C_7) = -132.1$

(*cf2*)

N							
C	1	B1					
C	1	B2	2	A1			
O	1	B3	2	A2	3	D1	0
C	2	B4	1	A3	4	D2	0
C	2	B5	1	A4	4	D3	0
C	3	B6	1	A5	4	D4	0
C	3	B7	1	A6	4	D5	0
N	7	B8	3	A7	1	D6	0
C	5	B9	2	A8	1	D7	0
C	7	B10	3	A9	1	D8	0
H	6	B11	2	A10	1	D9	0
H	6	B12	2	A11	1	D10	0
H	6	B13	2	A12	1	D11	0
H	8	B14	3	A13	1	D12	0
H	8	B15	3	A14	1	D13	0
H	8	B16	3	A15	1	D14	0
O	9	B17	7	A16	3	D15	0
H	10	B18	5	A17	2	D16	0
H	10	B19	5	A18	2	D17	0
H	10	B20	5	A19	2	D18	0
H	11	B21	7	A20	3	D19	0
H	11	B22	7	A21	3	D20	0
H	11	B23	7	A22	3	D21	0
Li	18	B24	9	A23	5	D22	0
Li	4	B25	1	A24	3	D23	0

2Li-(*cf1*)-TMePzDO						2Li-(*cf2*)-TMePzDO					
Bond-lengths (Å)		**Bond-angles (degree)**		**Dihedral angles (degree)**		**Bond-lengths (Å)**		**Bond-angles (degree)**		**Dihedral angles (degree)**	
B1	1.4261					**B1**	1.4196				
B2	1.4261	**A1**	115.42			**B2**	1.4228	**A1**	115.38		
B3	1.4388	**A2**	109.99	**D1**	125.1	**B3**	1.4170	**A2**	110.26	**D1**	126.2
B4	1.3387	**A3**	122.28	**D2**	126.2	**B4**	1.3404	**A3**	121.79	**D2**	133.5
B5	1.5017	**A4**	113.18	**D3**	-54.0	**B5**	1.4992	**A4**	113.00	**D3**	-50.8
B6	1.3387	**A5**	122.29	**D4**	-126.2	**B6**	1.3404	**A5**	122.47	**D4**	-132.1
B7	1.5017	**A6**	113.15	**D5**	54.1	**B7**	1.5046	**A6**	112.67	**D5**	52.4
B8	1.4261	**A7**	122.28	**D6**	1.1	**B8**	1.4196	**A7**	121.79	**D6**	-1.3
B9	1.5017	**A8**	124.56	**D7**	179.2	**B9**	1.5046	**A8**	124.69	**D7**	173.7
B10	1.5017	**A9**	124.54	**D8**	-179.1	**B10**	1.4992	**A9**	125.05	**D8**	-176.4
B11	1.0855	**A10**	112.20	**D9**	-161.1	**B11**	1.0862	**A10**	112.40	**D9**	-165.1
B12	1.0932	**A11**	109.56	**D10**	-42.1	**B12**	1.0925	**A11**	109.60	**D10**	-44.0
B13	1.0894	**A12**	111.45	**D11**	76.3	**B13**	1.0891	**A12**	110.52	**D11**	73.6
B14	1.0894	**A13**	111.43	**D12**	-75.9	**B14**	1.0954	**A13**	112.27	**D12**	-90.5
B15	1.0934	**A14**	109.54	**D13**	42.5	**B15**	1.0942	**A14**	109.40	**D13**	31.0
B16	1.0854	**A15**	112.21	**D14**	161.5	**B16**	1.0866	**A15**	112.64	**D14**	149.7
B17	1.4388	**A16**	109.99	**D15**	-126.2	**B17**	1.4168	**A16**	110.28	**D15**	133.6
B18	1.0894	**A17**	111.43	**D16**	-104.3	**B18**	1.0942	**A17**	109.41	**D16**	-144.4
B19	1.0934	**A18**	109.54	**D17**	137.2	**B19**	1.0954	**A18**	112.26	**D17**	94.1
B20	1.0854	**A19**	112.21	**D18**	18.2	**B20**	1.0866	**A19**	112.64	**D18**	-25.6
B21	1.0894	**A20**	111.45	**D19**	103.9	**B21**	1.0925	**A20**	109.60	**D19**	131.4
B22	1.0855	**A21**	112.20	**D20**	-18.7	**B22**	1.0861	**A21**	112.39	**D20**	10.3
B23	1.0932	**A22**	109.56	**D21**	-137.7	**B23**	1.0891	**A22**	110.51	**D21**	-111.0
B24	1.7439	**A23**	75.13	**D22**	115.7	**B24**	1.7194	**A23**	123.59	**D22**	-47.7
B25	1.7439	**A24**	75.13	**D23**	-115.7	**B25**	1.7195	**A24**	123.52	**D23**	-47.8

Table SI-7: Calculated structural parameters for the Doubly Reduced (DR) 2Li-TeMePzDO systems.