

Investigating the potential of pyrazine dioxide based-compounds as organic electrodes for batteries

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System	(3,-3) L(\vec{r}) CP type ^a	R(N), a.u. ^b	R(O), a.u. ^b	R(C), a.u. ^b	L(\vec{r}_{CP}), a.u.	$\rho(\vec{r}_{CP})$, a.u.
PZDO init.	<u>N</u> -C b.m.	0.785	-	1.773	2.497	0.540
	<u>N</u> -C b.m.	0.785	-	1.773	2.497	0.540
	<u>N</u> -O b.m.	0.800	1.624	-	2.149	0.513
PZDO cryst. init.	<u>N</u> -C b.m.	0.786	-	1.802	2.427	0.531
	<u>N</u> -C b.m.	0.786	-	1.803	2.425	0.531
	<u>N</u> -O b.m.	0.800	1.655	-	2.092	0.504
PZDO DR	<u>N</u> -C b.m.	0.805	-	1.873	1.961	0.482
	<u>N</u> -C b.m.	0.805	-	1.873	1.961	0.482
	<u>N</u> -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	<u>N</u> -C b.m.	0.805	-	1.864	1.974	0.484
	<u>N</u> -C b.m.	0.804	-	1.866	1.973	0.484
	<u>N</u> -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.	<u>N</u> -C b.m.	0.786	-	1.789	2.428	0.534
	<u>N</u> -C b.m.	0.786	-	1.789	2.428	0.534
	<u>N</u> -O b.m.	0.804	1.632	-	2.062	0.505
TeMePzDO cryst. init.	<u>N</u> -C b.m.	0.787	-	1.824	2.349	0.525
	<u>N</u> -C b.m.	0.787	-	1.824	2.350	0.524
	<u>N</u> -O b.m.	0.804	1.651	-	2.024	0.498
TeMePzDO DR	<u>N</u> -C b.m.	0.804	-	1.896	1.949	0.480
	<u>N</u> -C b.m.	0.804	-	1.896	1.949	0.480
	<u>N</u> -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	<u>N</u> -C b.m.	0.804	-	1.880	1.965	0.482
	<u>N</u> -C b.m.	0.804	-	1.881	1.957	0.482
	<u>N</u> -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 SI-1: Bonded maximum (b.m.) and lone pair (LP) maximum characterizing the (3, -3) critical point (CP) of the $L(\vec{r}) = -\nabla^2 \rho(\vec{r})$ distribution in the valence-shell charge concentration (VSCC) of the N atom for both the systems generated in the case of i) molecular SMD treatment (*i.e.* calculated thanks to the Gaussian package) and ii) the molecular complexes which are present in intercalated crystalline PZDO/TeMePzDO most stable relaxed phases (*i.e.* obtained through VASP calculations).

- a) The bold and underlined atom denotes that the listed critical point (CP) is located in the VSCC of this atom;
- b) the second-neighbour atom distance to the listed CP; for N-C or N-O bonds it is the C or O atoms of these bonds, while for the Nitrogen LP CP the almost equal distances of the CP to the N-bonded carbon and oxygen atoms is reported.

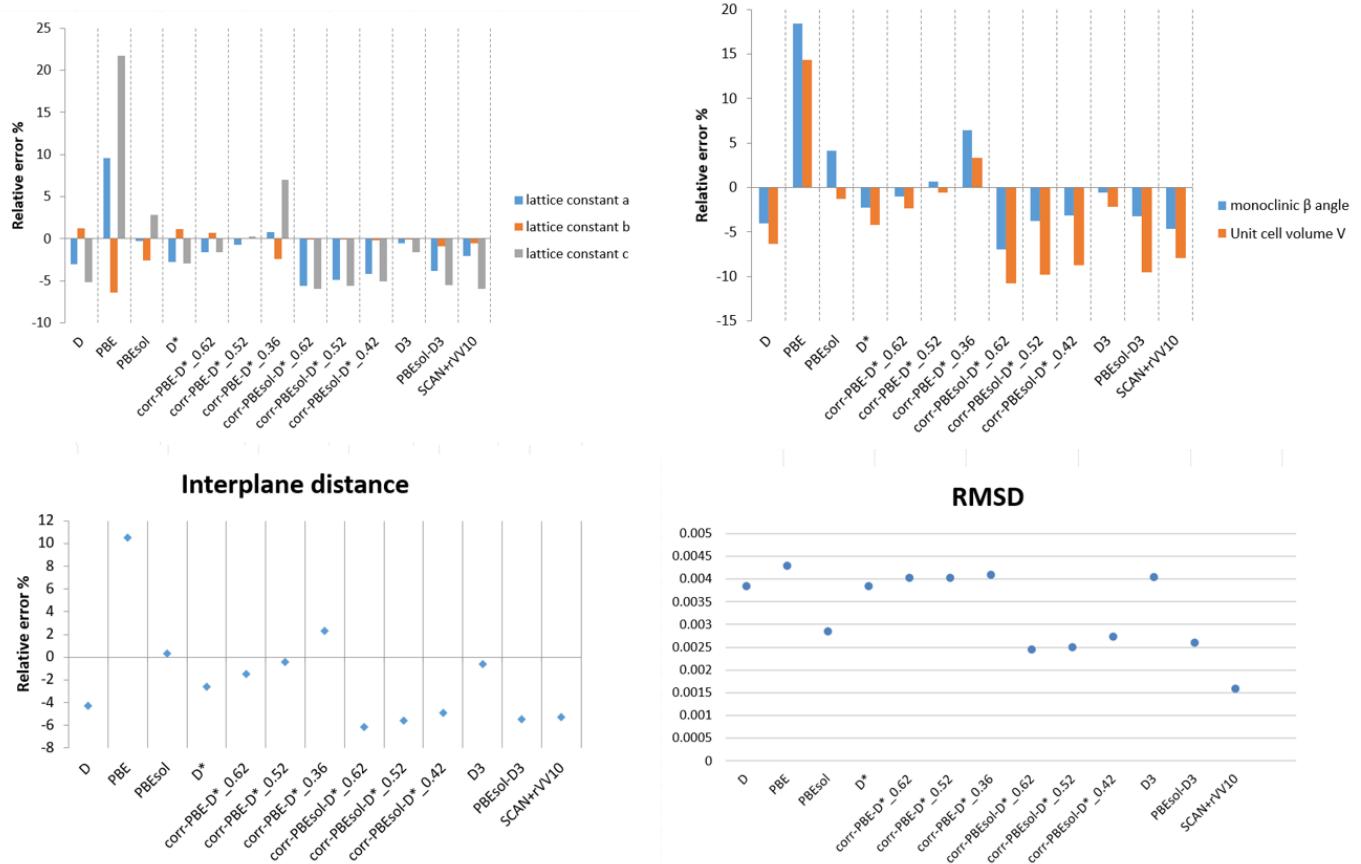


Figure SI-1: Relative errors (%) of DFT calculated values to experiment for the PZDO crystal: (a) for the optimized lattice parameters: a , b and c , and (b)

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.

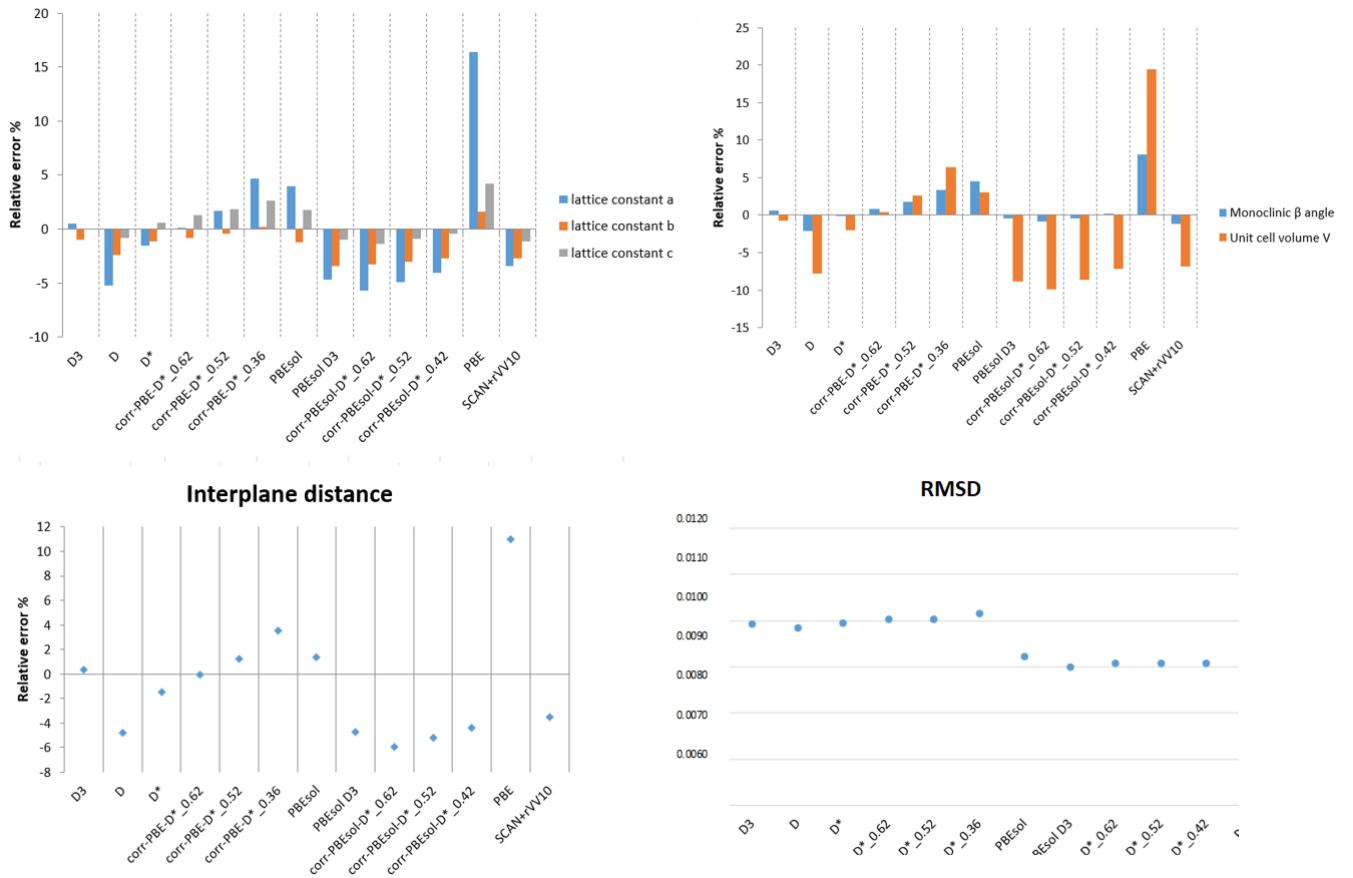


Figure SI-2: Relative errors (%) of DFT calculated values to experiment for the TeMePzDO crystal: (a)
for the optimized lattice parameters: *a*, *b* and *c*, and (b)
for the unit-cell volume *V* and the monoclinic angle β ; c) Relative errors (%) of DFT calculated values
to experiment for the inter-plane 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.

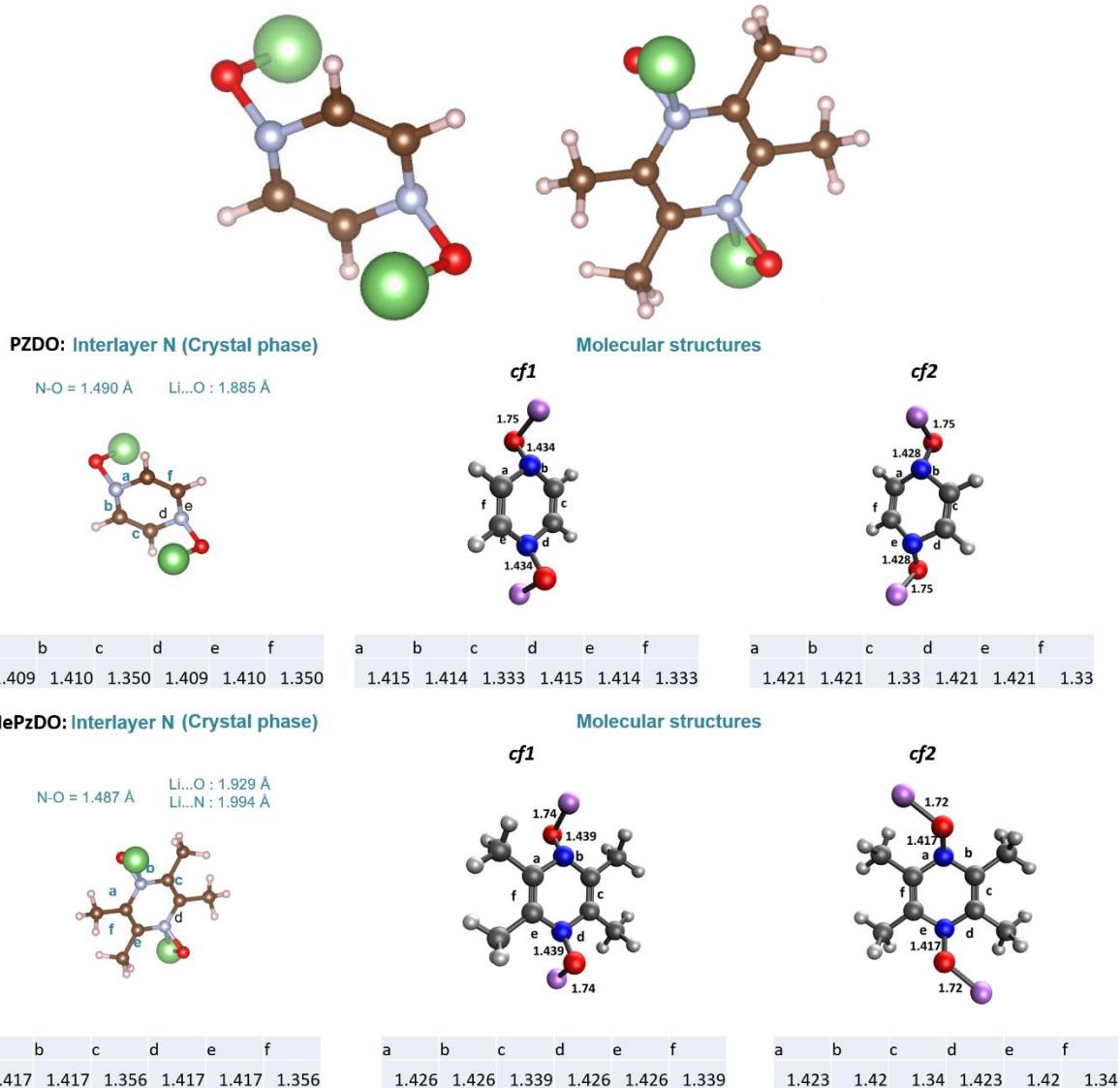


Figure SI-3: Top: relaxed molecular structure extracted from the most stable intercalated PZDO and TeMePzDO crystalline phases; middle and bottom: comparison of their bond length (left) with those of molecular complexes (middle and right corresponding to two distinct conformations, cf1 and cf2).

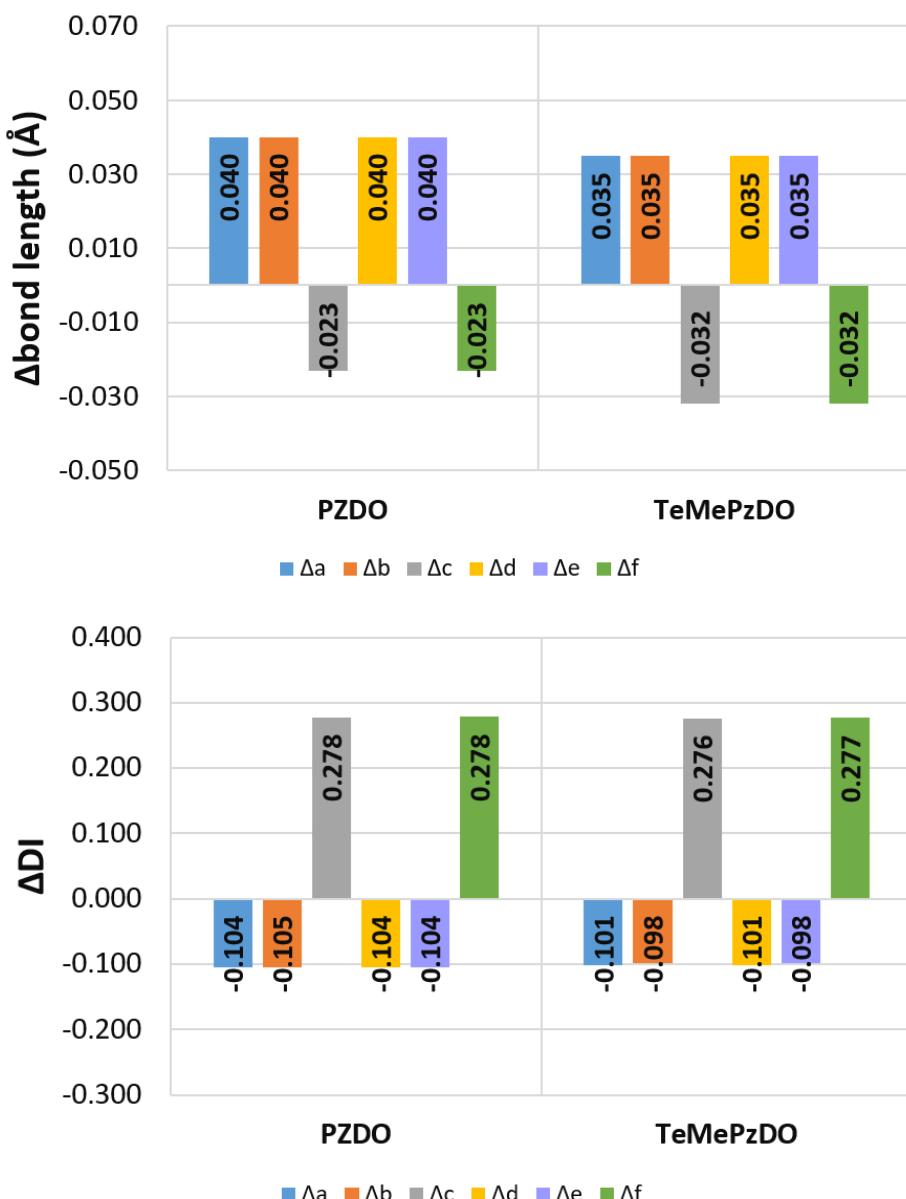


Figure SI-4: Top: Calculated bond length variations (Δ bond length) of each bond in the ring for the single (left) and double (right) reduction process characterizing molecular species in the intercalated crystalline structures; bottom: calculated DI variations (Δ DI) of each bond in the ring for the single (left) and double (right) reduction process in the intercalated crystalline structures.

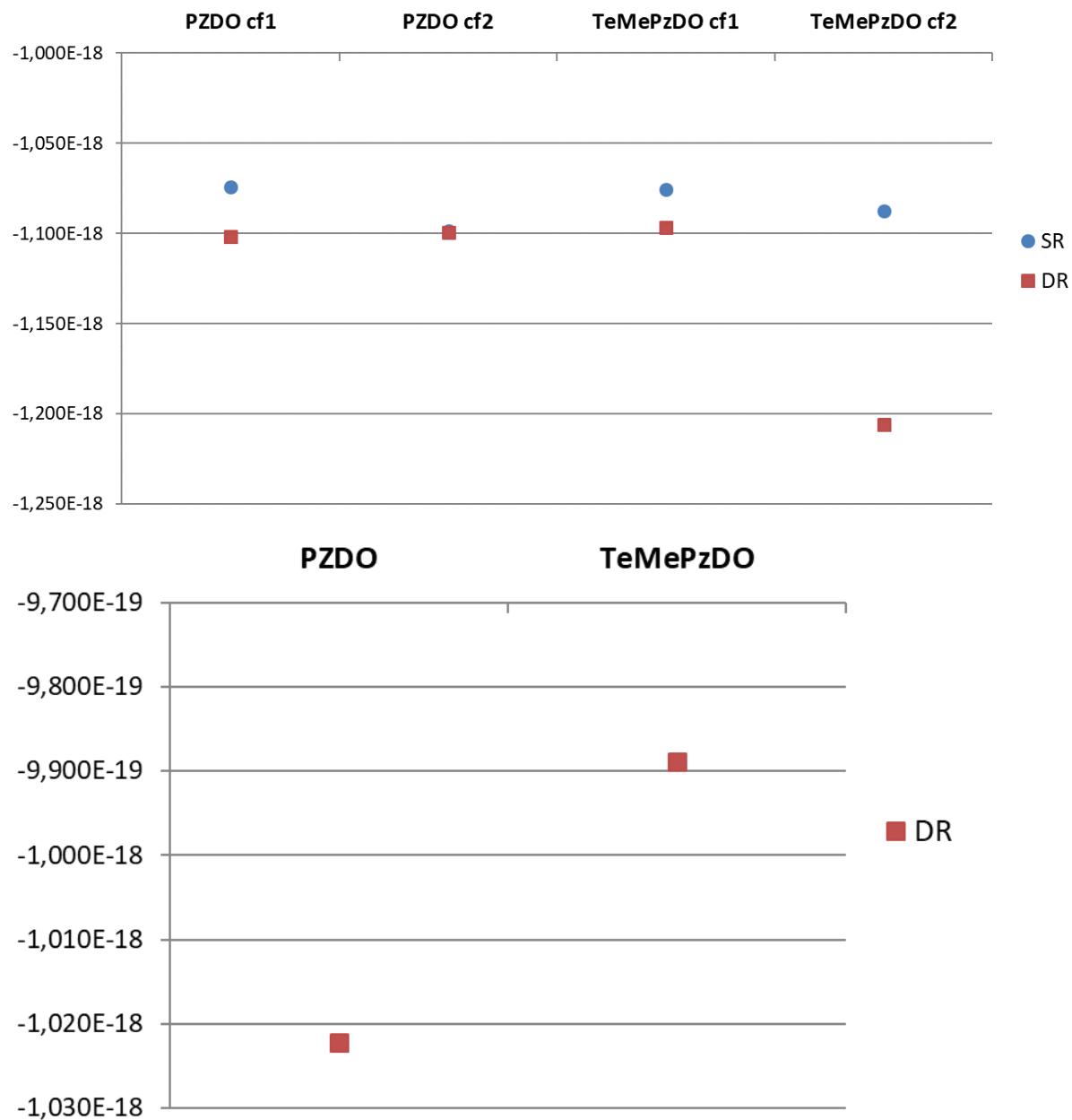
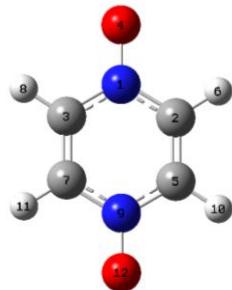


Figure SI-5: (a) Estimation of the electrostatic interaction energy (in Joule), between the Li^+ cations and the oxygen atoms: top: in the case of molecular species; bottom: for the same complexes, which are present in the intercalated crystal phases.

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

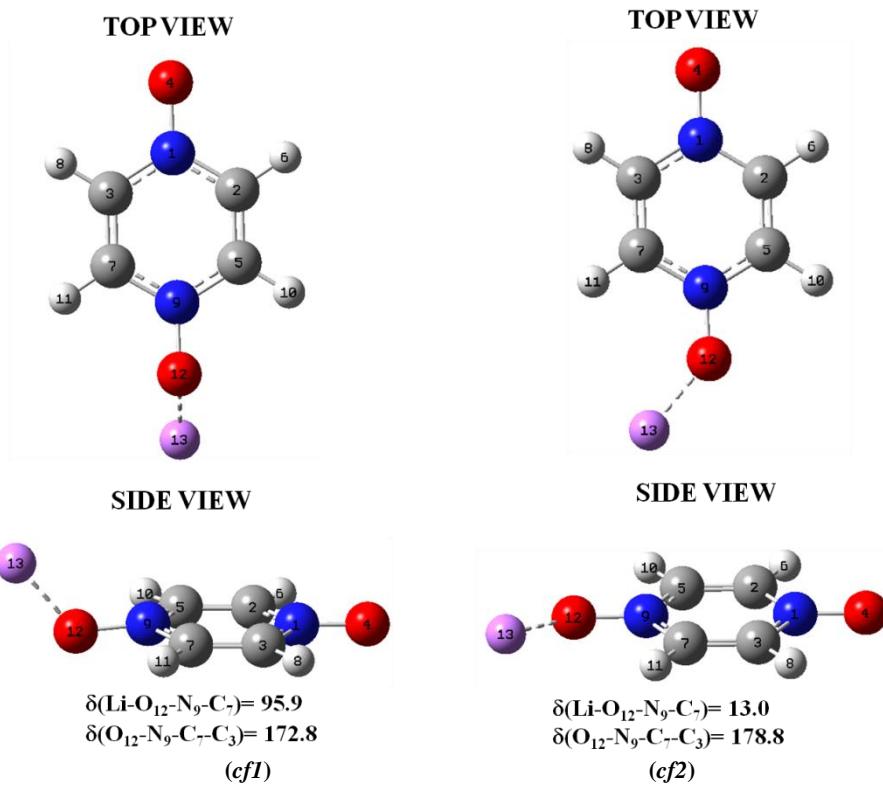


	N					
C	1	B1				
C	1	B2	2	A1		
O	1	B3	2	A2	3	D1
C	2	B4	1	A3	4	D2
H	2	B5	1	A4	4	D3
C	3	B6	1	A5	4	D4
H	3	B7	1	A6	4	D5
N	7	B8	3	A7	1	D6
H	5	B9	2	A8	1	D7
H	7	B10	3	A9	1	D8
O	9	B11	7	A10	3	D9

	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



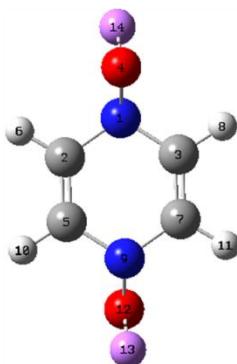
N					
C	1	B1			
C	1	B2	2	A1	
O	1	B3	2	A2	3
C	2	B4	1	A3	4
H	2	B5	1	A4	4
C	3	B6	1	A5	4
H	3	B7	1	A6	4
N	7	B8	3	A7	1
H	5	B9	2	A8	1
H	7	B10	3	A9	1
O	9	B11	7	A10	3
Li	12	B12	9	A11	7
					D10

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	B3	1.3169	A2	121.34
B4	1.3521	A3	121.27	B4	1.3520	A3	121.30
B5	1.0774	A4	116.04	B5	1.0773	A4	116.06
B6	1.3521	A5	121.27	B6	1.3524	A5	121.33
B7	1.0774	A6	116.04	B7	1.0774	A6	116.08
B8	1.3732	A7	120.95	B8	1.3733	A7	120.89
B9	1.0778	A8	122.63	B9	1.0777	A8	122.72
B10	1.0778	A9	122.63	B10	1.0782	A9	122.34
B11	1.3522	A10	120.44	B11	1.3428	A10	121.70
B12	1.7505	A11	124.77	B12	1.7284	A11	137.39
		D10	95.9			D10	13.0

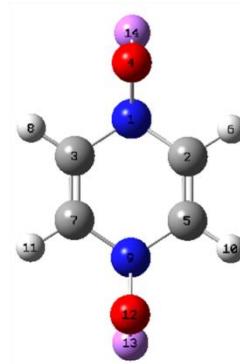
Table SI-3: Calculated structural parameters for Singly Reduced (SR) Li-PZDO systems.

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

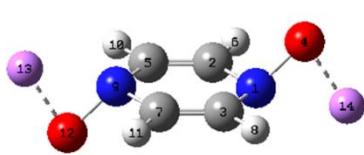
TOP VIEW



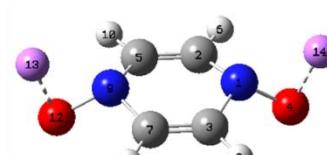
TOP VIEW



SIDE VIEW



SIDE VIEW



$$\begin{aligned} \delta(\text{Li}-\text{O}_{12}-\text{N}_9-\text{C}_7) &= 116.9 & \delta(\text{Li}-\text{O}_4-\text{N}_1-\text{C}_2) &= -116.9 \\ \delta(\text{O}_{12}-\text{N}_9-\text{C}_7-\text{C}_3) &= 127.7 & \delta(\text{O}_4-\text{N}_1-\text{C}_2-\text{C}_5) &= -127.7 \end{aligned}$$

(cf1)

$$\begin{aligned} \delta(\text{Li}-\text{O}_{12}-\text{N}_9-\text{C}_7) &= 117.6 & \delta(\text{Li}-\text{O}_4-\text{N}_1-\text{C}_2) &= 117.6 \\ \delta(\text{O}_{12}-\text{N}_9-\text{C}_7-\text{C}_3) &= 143.0 & \delta(\text{O}_4-\text{N}_1-\text{C}_2-\text{C}_5) &= 143.0 \end{aligned}$$

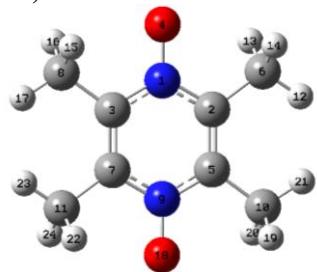
(cf2)

N		B1			
C	1	B2	2	A1	
O	1	B3	2	A2	3
C	2	B4	1	A3	4
H	2	B5	1	A4	4
C	3	B6	1	A5	4
H	3	B7	1	A6	4
N	7	B8	3	A7	1
H	5	B9	2	A8	1
H	7	B10	3	A9	1
O	9	B11	7	A10	3
Li	12	B12	9	A11	5
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)	Bond lengths (Å)	Bond 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



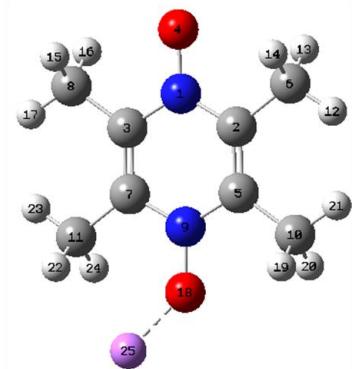
N					
C	1	B1			
C	1	B2	2	A1	
O	1	B3	2	A2	3
C	2	B4	1	A3	4
C	2	B5	1	A4	4
C	3	B6	1	A5	4
C	3	B7	1	A6	4
N	7	B8	3	A7	1
C	5	B9	2	A8	1
C	7	B10	3	A9	1
H	6	B11	2	A10	1
H	6	B12	2	A11	1
H	6	B13	2	A12	1
H	8	B14	3	A13	1
H	8	B15	3	A14	1
H	8	B16	3	A15	1
O	9	B17	7	A16	3
H	10	B18	5	A17	2
H	10	B19	5	A18	2
H	10	B20	5	A19	2
H	11	B21	7	A20	3
H	11	B22	7	A21	3
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

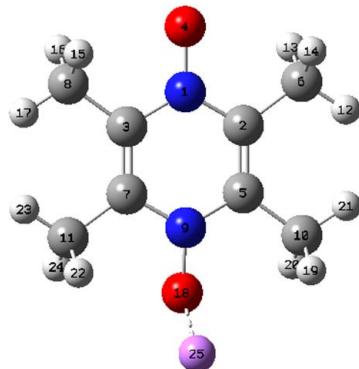
Table SI-5: Calculated structural parameters for the molecular (unreduced) TeMePzDO system.

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

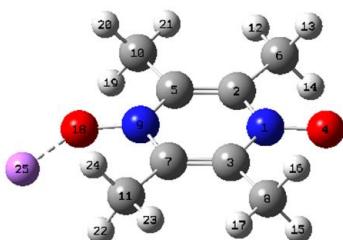
TOP VIEW



TOP VIEW

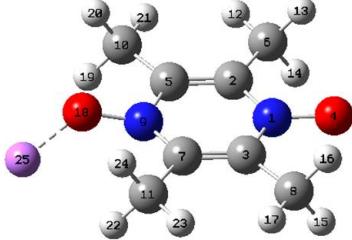


SIDE VIEW



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

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)

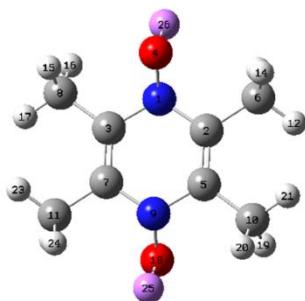
N				
C	1	B1		
C	1	B2	2	A1
O	1	B3	2	A2
C	2	B4	1	A3
C	2	B5	1	A4
C	3	B6	1	A5
C	3	B7	1	A6
N	7	B8	3	A7
C	5	B9	2	A8
C	7	B10	3	A9
H	6	B11	2	A10
H	6	B12	2	A11
H	6	B13	2	A12
H	8	B14	3	A13
H	8	B15	3	A14
H	8	B16	3	A15
O	9	B17	7	A16
H	10	B18	5	A17
H	10	B19	5	A18
H	10	B20	5	A19
H	11	B21	7	A20
H	11	B22	7	A21
H	11	B23	7	A22
Li	18	B24	9	A23
			5	D22

Li-(c1)-TeMePzDO						Li-(c2)-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

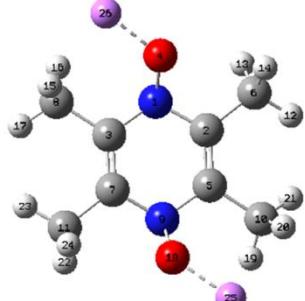
Table SI-6: Calculated structural parameters for the Singly Reduced (SR) 1Li-TeMePzDO systems.

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

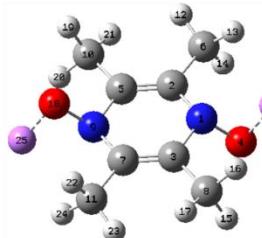
TOP VIEW



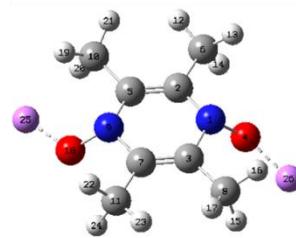
TOP VIEW



SIDE VIEW



SIDE VIEW



$\delta(\text{Li}-\text{O}_{18}-\text{N}_9-\text{C}_5)=115.7 \quad \delta(\text{Li}-\text{O}_4-\text{N}_1-\text{C}_2)=-115.7$
 $\delta(\text{O}_{18}-\text{N}_9-\text{C}_5-\text{C}_2)=-126.2 \quad \delta(\text{O}_4-\text{N}_1-\text{C}_3-\text{C}_7)=126.2$

(cf1)

$\delta(\text{Li}-\text{O}_{18}-\text{N}_9-\text{C}_5)=-47.7 \quad \delta(\text{Li}-\text{O}_4-\text{N}_1-\text{C}_2)=-47.8$
 $\delta(\text{O}_{18}-\text{N}_9-\text{C}_5-\text{C}_2)=-132.2 \quad \delta(\text{O}_4-\text{N}_1-\text{C}_3-\text{C}_7)=-132.1$

(cf2)

N		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.