

Supplementary Information

A Computational Study of the Complex Dichlorobis(pyrazinamido)platinum(II), [PtCl₂(PZA)₂], Applying a Mixed-Level Factorial Design

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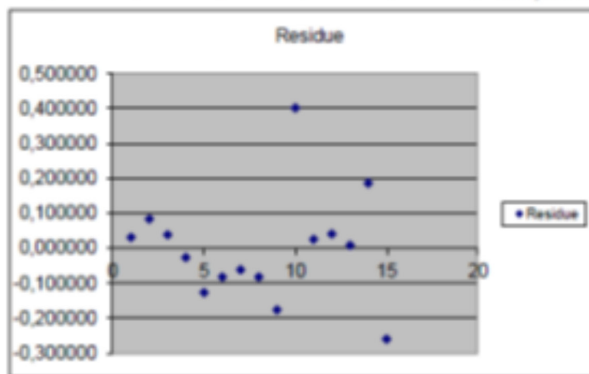
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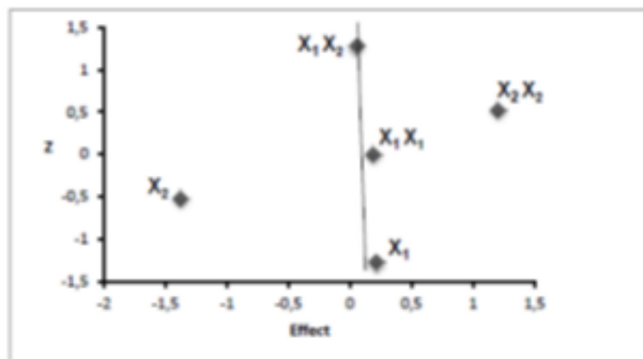
Excel sheet including coefficient errors and graphic of residues

exp	M	x1	x2	x1x1	x2x2	x1x2	energy values (responses)			predictability
1	1	1	-1	-1	1	1	1 -1904,240515	b0	-1905,57	-1904,271690
2	1	-0,5	-1	0,25	1	0,5	0,5 -1904,226578	b1	0,107829	-1904,310052
3	1	0	-1	0	1	0	0 -1904,257614	b2	-0,67779	-1904,296490
4	1	0,5	-1	0,25	1	-0,5	-0,5 -1904,257613	b11	0,103847	-1904,231005
5	1	1	-1	-1	1	1	-1 -1904,240515	b22	0,595409	-1904,113597
6	1	-1	0	1	0	0	0 -1905,655901	b12	0,028782	-1905,573673
7	1	-0,5	0	0,25	0	0	0 -1905,658634			-1905,597644
8	1	0	0	0	0	0	0 -1905,651833			-1905,569691
9	1	0,5	0	0,25	0	0	0 -1905,666190			-1905,489815
10	1	1	0	1	0	0	0 -1904,956282			-1905,358016
11	1	-1	1	1	1	-1	-1 -1905,659706			-1905,684837
12	1	-0,5	1	0,25	1	-0,5	-0,5 -1905,653522			-1905,694417
13	1	0	1	0	1	0	0 -1905,643420			-1905,652073
14	1	0,5	1	0,25	1	0,5	0,5 -1905,372054			-1905,557806
15	1	1	1	1	1	1	1 -1905,672048			-1905,411616



b0	-1905,56969
b1	0,1078288
b2	-0,6777915
b11	0,103846857
b22	0,5954094
b12	0,0287819

	coef	effect	order	effect	probability	Central point	Z		effect	Z	
b0	-1905,57	-1905,57	1	-1,37174	0	20	10	-1,28	0,1 X1	0,217034	-1,28
b2	-0,68587	-1,37174	2	0,0555	20	40	30	-1,88	0,3 x2	-1,37174	-0,52
b12	0,02775	0,0555	3	0,192309	40	60	50	0	0,5 x1x1	0,192309	0
b11	0,096155	0,192309	4	0,217034	60	80	70	1,88	0,7 x2x2	1,206972	0,52
b1	0,108517	0,217034	5	1,206972	80	100	90	1,28	0,9 x1x2	0,0555	1,28
b22	0,603486	1,206972									



exp	Residue	response	predictability	SQ _{re}	SQ _i	SQ _o	R ²
1	0,031175	-1904,240515	-1904,27169	5,89537433	0,340702001	6,236076332	0,945365967
2	0,083474	-1904,226578	-1904,31005				
3	0,038876	-1904,257614	-1904,29649				
4	-0,026608	-1904,257613	-1904,23101	1,179074866	0,037855778	0,445434024	
5	-0,126918	-1904,240515	-1904,1136				
6	-0,082228	-1905,655901	-1905,57367				
7	-0,060990	-1905,658634	-1905,59764				
8	-0,082142	-1905,651833	-1905,56969				
9	-0,176375	-1905,666190	-1905,48982				
10	0,401734	-1904,956282	-1905,35802				
11	0,025131	-1905,659706	-1905,68484				
12	0,040895	-1905,653522	-1905,69442				
13	0,008653	-1905,643420	-1905,65207				
14	0,185752	-1905,372054	-1905,55781				
15	-0,260432	-1905,672048	-1905,41162				

	x2							
	1	0,8	0,6	0,4	0,2	0	-0,2	
	-1	-1905,684837	-1905,757870	-1905,783270	-1905,761037	-1905,691172	-1905,573673	-1905,408542
	-0,8	-1905,694900	-1905,769084	-1905,795635	-1905,774554	-1905,705839	-1905,589492	-1905,425513
	-0,6	-1905,696855	-1905,771990	-1905,799691	-1905,779762	-1905,712199	-1905,597004	-1905,434175
	-0,4	-1905,690102	-1905,766589	-1905,795443	-1905,776664	-1905,710252	-1905,596207	-1905,434530
	-0,2	-1905,675242	-1905,752880	-1905,782885	-1905,765257	-1905,699996	-1905,587103	-1905,426577
x1	0	-1905,652073	-1905,730863	-1905,762019	-1905,745542	-1905,681433	-1905,569691	-1905,410317
	0,2	-1905,620597	-1905,700538	-1905,732845	-1905,717520	-1905,654562	-1905,543972	-1905,385748
	0,4	-1905,580814	-1905,661905	-1905,695364	-1905,681190	-1905,619384	-1905,509944	-1905,352872
	0,6	-1905,532722	-1905,614965	-1905,649575	-1905,636553	-1905,575897	-1905,467609	-1905,311688
	0,8	-1905,476323	-1905,559717	-1905,595479	-1905,583607	-1905,524103	-1905,416966	-1905,262197
	1	-1905,411616	-1905,496161	-1905,533074	-1905,522354	-1905,464001	-1905,358016	-1905,204397

