

ELECTRONIC SUPPLEMENTARY INFORMATION

Coupling of Platinated Triguanides with Platinum-Activated Nitriles as a Novel Strategy for Generation of Dimetallic Systems

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Table S1. Crystallographic data for **3'a**•2CH₂Cl₂ and **2a**•2CDCl₃.

Compound	3'a •2CH ₂ Cl ₂	2a •2CDCl ₃
Formula	C ₂₄ H ₃₃ Cl ₄ N ₉ Pt ₂ , 6(CH ₂ Cl ₂)	C ₂₅ H ₃₅ Cl ₆ N ₉ Pt ₂ , 2(CDCl ₃)
Crystal System	Monoclinic	Monoclinic
<i>a</i> (Å)	32.9496(14)	12.0973(5)
<i>b</i> (Å)	15.7777(5)	13.5538(5)
<i>c</i> (Å)	17.6434(6)	26.8946(19)
α (°)	90	90.00
β (°)	116.753(4)	98.307(5)
γ (°)	90	90.00
<i>V</i> (Å ³)	8190.4(6)	4363.5(4)
Molecular weight	990.19	1300.21
Space group	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>n</i>
μ (mm ⁻¹)	7.126	7.173
Temperature (K)	100(2)	100(2)
<i>Z</i>	8	4
<i>D</i> _{calc} (g/cm ³)	1.606	1.979
Crystal size (mm ³)	0.23×0.18×0.12	0.25×0.19×0.16
Radiation	MoK α	MoK α
Total reflections	62905	42248
Unique reflections	9356	8537
Angle range 2 θ (°)	5.16–55.00	5.2–52.00
Reflections with $ F_o \geq 4\sigma_F$	5721	5610
<i>R</i> _{int}	0.0709	0.0839
<i>R</i> _{σ}	0.0565	0.0988
<i>R</i> ₁ ($ F_o \geq 4\sigma_F$)	0.0713	0.0947
<i>wR</i> ₂ ($ F_o \geq 4\sigma_F$)	0.1703	0.2010
<i>R</i> ₁ (all data)	0.1244	0.1435
<i>wR</i> ₂ (all data)	0.1978	0.2343
<i>S</i>	1.059	1.046
$\rho_{\min}$, $\rho_{\max}$, e/Å ³	–0.570, 1.576	–3.25, 5.10
$R_1 = \Sigma F_o - F_c /\Sigma F_o $; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = (F_o^2 + 2F_c^2)/3$; $s = \{\Sigma[w(F_o^2 - F_c^2)]/(n - p)\}^{1/2}$ where <i>n</i> is the number of reflections and <i>p</i> is the number of refinement parameters.		

Table S2. Bond Lengths for **3'a**•2CH₂Cl₂.

Atom	Atom	Length, Å	Atom	Atom	Length, Å
Pt1	Cl1	2.285(4)	N8	C22	1.318(14)
Pt1	N1	1.953(13)	N8	C23	1.469(15)
Pt1	N2	2.007(9)	N8	C24	1.405(16)
Pt1	Cl2A	2.310(8)	N9	C3	1.378(14)
Pt1	Cl2B	2.20(3)	N9	C15	1.264(12)
Pt2	Cl3	2.298(3)	C1	C2	1.514(15)
Pt2	Cl4	2.296(3)	C3	C4	1.537(17)
Pt2	N3	2.024(9)	C4	C5	1.51(2)
Pt2	N4	2.026(9)	C9	C10	1.378(14)
N1	C1	1.206(13)	C9	C14	1.402(14)
N2	C3	1.256(13)	C10	C11	1.375(16)
N3	C6	1.297(13)	C11	C12	1.403(19)
N4	C22	1.345(14)	C12	C13	1.361(19)
N5	C6	1.344(13)	C13	C14	1.327(15)
N5	C7	1.432(15)	C16	C17	1.374(14)
N5	C8	1.440(14)	C16	C21	1.390(14)
N6	C6	1.436(12)	C17	C18	1.353(15)
N6	C9	1.470(12)	C18	C19	1.396(17)
N6	C15	1.349(13)	C19	C20	1.395(16)
N7	C15	1.408(12)	C20	C21	1.377(15)
N7	C16	1.450(12)	Cl5	C25	2.01(5)
N7	C22	1.412(13)			

Table S3. Bond Angles for **3'a**•2CH₂Cl₂.

Atom	Atom	Atom	Angle, °	Atom	Atom	Atom	Angle, °
Cl1	Pt1	Cl2A	176.6(4)	N1	C1	C2	174(2)
N1	Pt1	Cl1	91.3(5)	N2	C3	N9	119.3(10)
N1	Pt1	N2	174.6(5)	N2	C3	C4	120.9(12)
N1	Pt1	Cl2A	89.1(5)	N9	C3	C4	119.6(10)
N1	Pt1	Cl2B	93.0(11)	C5	C4	C3	114.5(13)
N2	Pt1	Cl1	91.6(3)	N3	C6	N5	125.7(9)
N2	Pt1	Cl2A	87.7(3)	N3	C6	N6	117.6(10)
N2	Pt1	Cl2B	85.8(10)	N5	C6	N6	116.6(9)
Cl2B	Pt1	Cl1	160.2(17)	C10	C9	N6	120.3(9)
Cl4	Pt2	Cl3	91.86(13)	C10	C9	C14	120.8(9)
N3	Pt2	Cl3	179.3(3)	C14	C9	N6	118.9(9)
N3	Pt2	Cl4	88.7(3)	C11	C10	C9	118.7(11)
N3	Pt2	N4	93.3(4)	C10	C11	C12	120.1(12)
N4	Pt2	Cl3	86.1(3)	C13	C12	C11	118.5(12)
N4	Pt2	Cl4	177.0(3)	C14	C13	C12	123.1(12)
C1	N1	Pt1	177.0(18)	C13	C14	C9	118.6(11)
C3	N2	Pt1	132.3(9)	N6	C15	N7	116.2(8)
C6	N3	Pt2	127.5(7)	N9	C15	N6	119.6(9)
C22	N4	Pt2	130.0(8)	N9	C15	N7	124.1(10)
C6	N5	C7	120.7(10)	C17	C16	N7	121.7(9)
C6	N5	C8	124.3(10)	C17	C16	C21	121.7(9)
C7	N5	C8	113.6(10)	C21	C16	N7	116.5(9)
C6	N6	C9	117.0(9)	C18	C17	C16	119.5(10)
C15	N6	C6	117.1(8)	C17	C18	C19	120.6(10)
C15	N6	C9	121.4(8)	C20	C19	C18	119.5(10)
C15	N7	C16	119.5(8)	C21	C20	C19	120.0(11)
C15	N7	C22	119.7(8)	C20	C21	C16	118.6(10)
C22	N7	C16	117.6(7)	N4	C22	N7	117.5(10)
C22	N8	C23	119.9(11)	N8	C22	N4	124.3(10)
C22	N8	C24	123.8(10)	N8	C22	N7	118.1(10)
C24	N8	C23	116.0(11)	Cl5 ¹	C25	Cl5	119(5)
C15	N9	C3	126.1(9)				

¹-X,+Y,1/2-Z

Table S4. Bond Lengths for **2a**•2CDCl₃.

Atom	Atom	Length, Å	Atom	Atom	Length, Å
Pt1	Cl1	2.313(7)	N6	C15	1.39(2)
Pt1	Cl2	2.320(6)	N7	C15	1.418(17)
Pt1	N1	1.963(19)	N7	C16	1.436(18)
Pt1	N2	1.993(14)	N7	C22	1.381(19)
Pt2	Cl3	2.302(5)	N8	C22	1.300(19)
Pt2	Cl4	2.319(6)	N8	C23	1.50(2)
Pt2	Cl5	2.324(4)	N8	C24	1.46(2)
Pt2	Cl6	2.319(4)	N9	C3	1.37(2)
Pt2	N3	2.055(15)	N9	C15	1.28(2)
Pt2	N4	2.035(16)	C1	C2	1.44(3)
Cl7	C26	1.59(3)	C2	C25	1.39(3)
Cl8	C26	1.79(3)	C3	C4	1.47(2)
Cl9	C26	1.774(18)	C4	C5	1.54(3)
Cl10	C27	1.74(4)	C9	C10	1.36(2)
Cl11	C27	1.71(3)	C9	C14	1.36(2)
Cl12	C27	1.75(3)	C10	C11	1.38(2)
N1	C1	1.15(3)	C11	C12	1.37(2)
N2	C3	1.30(2)	C12	C13	1.35(3)
N3	C6	1.303(19)	C13	C14	1.40(2)
N4	C22	1.35(2)	C16	C17	1.37(2)
N5	C6	1.35(2)	C16	C21	1.38(2)
N5	C7	1.41(2)	C17	C18	1.40(2)
N5	C8	1.45(2)	C18	C19	1.38(2)
N6	C6	1.41(2)	C19	C20	1.36(2)
N6	C9	1.455(18)	C20	C21	1.38(2)

Table S5. Bond Angles for **2a**•2CDCl₃.

Atom	Atom	Atom	Angle, °	Atom	Atom	Atom	Angle, °
Cl1	Pt1	Cl2	175.5(3)	N1	C1	C2	175(3)
N1	Pt1	Cl1	90.9(7)	C25	C2	C1	103(3)
N1	Pt1	Cl2	90.0(7)	N2	C3	N9	116.3(15)
N1	Pt1	N2	177.5(8)	N2	C3	C4	125.4(16)
N2	Pt1	Cl1	91.6(4)	N9	C3	C4	117.8(15)
N2	Pt1	Cl2	87.5(4)	C3	C4	C5	111.7(16)
Cl3	Pt2	Cl4	91.9(2)	N3	C6	N5	121.9(15)
Cl3	Pt2	Cl5	91.18(18)	N3	C6	N6	121.1(15)
Cl3	Pt2	Cl6	87.80(15)	N5	C6	N6	116.9(13)
Cl4	Pt2	Cl5	90.9(2)	C10	C9	N6	119.1(14)
Cl6	Pt2	Cl4	89.99(18)	C14	C9	N6	119.8(14)
Cl6	Pt2	Cl5	178.7(2)	C14	C9	C10	121.0(14)
N3	Pt2	Cl3	174.5(4)	C9	C10	C11	119.3(15)
N3	Pt2	Cl4	86.5(4)	C12	C11	C10	119.1(16)
N3	Pt2	Cl5	83.6(4)	C13	C12	C11	122.3(15)
N3	Pt2	Cl6	97.5(4)	C12	C13	C14	118.0(16)
N4	Pt2	Cl3	84.7(4)	C9	C14	C13	120.0(16)
N4	Pt2	Cl4	176.1(4)	N6	C15	N7	115.7(13)
N4	Pt2	Cl5	87.4(4)	N9	C15	N6	119.8(13)
N4	Pt2	Cl6	91.7(4)	N9	C15	N7	124.3(15)
N4	Pt2	N3	96.8(5)	C17	C16	N7	118.6(13)
C1	N1	Pt1	178(3)	C17	C16	C21	120.9(13)
C3	N2	Pt1	130.2(13)	C21	C16	N7	120.4(12)
C6	N3	Pt2	137.0(12)	C16	C17	C18	120.2(14)
C22	N4	Pt2	127.8(13)	C19	C18	C17	118.6(14)
C6	N5	C7	121.3(16)	C20	C19	C18	120.4(16)
C6	N5	C8	123.0(14)	C19	C20	C21	121.5(16)
C7	N5	C8	114.7(16)	C20	C21	C16	118.1(14)
C6	N6	C9	117.1(12)	N4	C22	N7	117.1(13)
C15	N6	C6	118.7(12)	N8	C22	N4	122.1(14)
C15	N6	C9	121.2(13)	N8	C22	N7	120.7(13)
C15	N7	C16	118.7(12)	Cl7	C26	Cl8	111.8(16)
C22	N7	C15	119.5(12)	Cl7	C26	Cl9	112.5(16)
C22	N7	C16	120.8(11)	Cl9	C26	Cl8	101.4(14)
C22	N8	C23	121.3(14)	Cl10	C27	Cl12	112.3(16)
C22	N8	C24	123.4(13)	Cl11	C27	Cl10	110.6(18)
C24	N8	C23	115.1(14)	Cl11	C27	Cl12	110.8(16)
C15	N9	C3	125.4(13)				

Table S6. Calculated total energies, enthalpies, Gibbs free energies (in Hartree) and entropies (in cal/mol•K) in gas phase (E_g , H_g , G_g , S_g) and CHCl_3 solution (E_s , H_s , G_s , S_s). The values for ΔG of solvation calculated as $G_g - G_s$ are given in kcal/mol.

Compound	E_g (6-31G(d))	E_s (6-31G(d))	H_g (6-31G(d))	H_s (6-31G(d))	S_g (6-31G(d))	S_s (6-31G(d))	G_g (6-31G(d))	G_s (6-31G(d))	ΔG_{solv}
[Pt ^{II} R]	-1305.410811	-1305.443917	-1305.298316	-1305.331638	126.82	123.20	-1305.358570	-1305.390173	19.83
[Pt ^{IV} R]	-2225.789057	-2225.831324	-2225.670132	-2225.712813	143.39	144.08	-2225.738261	-2225.781271	26.99
1	-2162.214703	-2162.274322	-2161.748315	-2161.806805	200.25	196.19	-2161.843459	-2161.900021	35.49
2'	-4388.049581	-4388.137235	-4387.460454	-4387.547490	292.60	282.24	-4387.599477	-4387.681592	51.53
2	-4388.064820	-4388.144223	-4387.475235	-4387.554125	287.14	279.30	-4387.611663	-4387.686828	47.17
3	-3467.664567	-3467.743137	-3467.081617	-3467.159546	272.94	267.22	-3467.211301	-3467.286513	47.20
4	-3082.616259	-3082.676683	-3082.143108	-3082.203136	211.21	210.69	-3082.243462	-3082.303242	37.51
5	-5308.453281	-5308.538439	-5307.856976	-5307.942018	297.56	292.81	-5307.998354	-5308.081143	51.95

Table S7. Calculated total reaction energies (ΔE), enthalpies, and Gibbs free energies of the following processes (ΔH and ΔG) (in kcal/mol) for the gas phase and CHCl_3 solution (in parentheses).

Process	ΔE	ΔH	ΔG
$[\text{Pt}^{\text{IV}}\text{R}] + \mathbf{1} \rightarrow [\text{Pt}^{\text{II}}\text{R}] + \mathbf{4}$	−14.63 (−9.38)	−14.42 (−9.51)	−12.75 (−7.61)
$[\text{Pt}^{\text{II}}\text{R}] + \mathbf{4} \rightarrow \mathbf{2}$	−23.69 (−14.82)	−21.22 (−12.14)	−6.04 (4.13)
$[\text{Pt}^{\text{IV}}\text{R}] + \mathbf{1} \rightarrow \mathbf{2}'$	−28.75 (−19.82)	−26.36 (−17.49)	−11.14 (−0.19)
$\mathbf{2}' \rightarrow \mathbf{2}$	−9.56 (−4.39)	−9.28 (−4.16)	−7.65 (−3.29)
$\mathbf{2} + \mathbf{2} \rightarrow \mathbf{3} + \mathbf{5}$	7.40 (4.31)	7.45 (4.20)	8.58 (3.77)
$\mathbf{1} + \mathbf{2} \rightarrow \mathbf{3} + \mathbf{4}$	−0.82 (−0.80)	−0.74 (−1.10)	0.23 (−1.82)
$\mathbf{4} + \mathbf{2} \rightarrow \mathbf{5} + \mathbf{1}$	8.22 (5.11)	8.19 (5.29)	8.35 (5.59)
$\mathbf{4} + [\text{Pt}^{\text{IV}}\text{R}] \rightarrow \mathbf{5}$	−30.10 (−19.10)	−27.44 (−16.36)	−10.44 (2.11)
$[\text{Pt}^{\text{II}}\text{R}] + \mathbf{5} \rightarrow [\text{Pt}^{\text{IV}}\text{R}] + \mathbf{2}$	6.41 (4.27)	6.23 (4.22)	4.39 (2.02)

Table S8. Cartesian atomic coordinates of the calculated equilibrium structures in gas phase and CHCl₃ solution (subscripts _(g) and _(s), respectively). Nuclear charges of elements are shown in the second column.

Structure	Charge	X	Y	Z
1_(g)				
	78	−1.984699	0.054312	0.300757
	17	−4.041876	−0.325536	−0.770475
	17	−2.694053	2.021671	1.386633
	7	−0.224714	0.330028	1.328443
	1	−0.364188	0.285688	2.332942
	7	−1.400941	−1.669890	−0.619539
	1	−2.206464	−2.176779	−0.982420
	7	1.683462	1.572553	1.863310
	7	1.305865	0.915142	−0.363823
	7	0.698740	0.137263	−2.467461
	1	0.543622	−0.721629	−2.995641
	7	−0.072642	−3.536653	−1.149962
	7	0.923796	−1.440358	−0.674632
	6	0.889762	0.908058	0.978950
	6	1.123310	2.076193	3.113553
	1	0.064982	2.314721	2.978177
	1	1.653207	2.994116	3.386389
	1	1.236584	1.357917	3.939048
	1	3.619746	1.359967	2.628423
	6	3.128296	1.695294	1.706838
	1	3.417788	2.733774	1.507435
	1	3.469989	1.065226	0.887648
	6	1.564123	2.218543	−0.953508
	6	0.596465	3.220223	−0.850511
	1	−0.351203	3.014971	−0.358535
	6	0.853525	4.474675	−1.405423
	1	0.101212	5.254313	−1.328520
	6	2.056502	4.720384	−2.069601
	1	2.247968	5.696609	−2.506439
	6	3.011859	3.707271	−2.178304
	1	3.947703	3.891433	−2.698739
	6	2.769701	2.455059	−1.615173
	1	3.505709	1.660465	−1.696840
	6	0.930467	−0.122234	−1.245691
	6	−0.238946	−2.212136	−0.829021
	6	0.960721	−3.983807	−2.081341
	1	1.740155	−3.229677	−2.176559
	1	0.531245	−4.176687	−3.074978
	1	1.416194	−4.909343	−1.713524
	1	−0.806640	−5.469493	−0.898695

	6	-1.196378	-4.450995	-0.987096
	1	-1.890942	-4.422494	-1.840226
	1	-1.747455	-4.206205	-0.075530
	6	2.032232	-1.905328	0.097376
	6	3.339678	-1.639488	-0.332502
	1	3.499222	-1.091259	-1.256819
	6	4.425976	-2.088382	0.418957
	1	5.435488	-1.876070	0.077874
	6	4.219591	-2.823954	1.587541
	1	5.066651	-3.182122	2.165180
	6	2.915882	-3.098407	2.006767
	1	2.744370	-3.666521	2.916879
	6	1.823347	-2.634082	1.275195
	1	0.810737	-2.829482	1.613389
1_(s)				
	78	-2.052090	0.308578	0.229466
	17	-4.136198	0.095981	-0.892910
	17	-2.736192	2.302283	1.327872
	7	-0.299658	0.454050	1.287662
	1	-0.472230	0.396372	2.286684
	7	-1.577872	-1.457039	-0.678316
	1	-2.403716	-1.913292	-1.058014
	7	1.758196	1.366034	1.923418
	7	1.383908	0.806640	-0.330703
	7	0.757274	0.080001	-2.451952
	1	0.553649	-0.770569	-2.979196
	7	-0.444538	-3.460869	-1.113879
	7	0.759712	-1.485821	-0.635802
	6	0.910932	0.858161	0.993231
	6	1.249414	1.815732	3.216896
	1	0.267609	2.280497	3.100249
	1	1.938957	2.564988	3.615116
	1	1.180076	0.990940	3.940294
	1	3.574340	0.728898	2.746355
	6	3.212785	1.230395	1.840832
	1	3.691575	2.212727	1.766021
	1	3.492909	0.624913	0.981798
	6	1.968090	2.004871	-0.902830
	6	1.279497	3.217873	-0.837633
	1	0.296236	3.262043	-0.380705
	6	1.856390	4.367571	-1.380678
	1	1.318108	5.309697	-1.327409
	6	3.104412	4.304122	-2.002517
	1	3.546727	5.199338	-2.430825
	6	3.781321	3.083802	-2.076815
	1	4.752102	3.025563	-2.561371
	6	3.219040	1.934853	-1.522050
	1	3.744656	0.986213	-1.571476
	6	0.931165	-0.189283	-1.220080

	6	-0.467892	-2.132937	-0.824928
	6	0.607915	-4.078362	-1.922319
	1	1.383580	-3.354647	-2.165610
	1	0.174471	-4.451691	-2.858463
	1	1.060437	-4.918231	-1.384290
	1	-1.362426	-5.304687	-0.806032
	6	-1.655556	-4.262649	-0.962489
	1	-2.296061	-4.213552	-1.854090
	1	-2.226417	-3.927766	-0.092728
	6	1.809824	-2.082907	0.138278
	6	3.137156	-1.980552	-0.298878
	1	3.361621	-1.464894	-1.227834
	6	4.164086	-2.556468	0.449958
	1	5.190169	-2.469590	0.103529
	6	3.874506	-3.258230	1.622086
	1	4.674249	-3.715621	2.197431
	6	2.548609	-3.372792	2.046376
	1	2.311926	-3.916652	2.956763
	6	1.516765	-2.780063	1.317720
	1	0.491194	-2.860328	1.663137
$2_{(g)}$				
	78	-2.006322	-1.824016	-0.837395
	17	-0.780971	-3.692755	-1.562416
	17	-3.849323	-2.340677	-2.226762
	7	-3.223070	-0.280820	-0.124605
	7	-0.381077	-1.463623	0.408980
	7	-4.458191	1.685360	-0.114451
	7	-2.109771	1.808396	-0.150503
	7	0.183251	1.698733	-0.236666
	7	0.288814	-1.164988	2.627200
	7	-0.943096	0.518015	1.515861
	6	-3.271029	1.023073	-0.126274
	6	-5.670642	1.028416	-0.601866
	6	-4.659370	2.961191	0.568819
	6	-2.067325	2.952415	-1.047834
	6	-2.373585	2.786436	-2.398516
	6	-2.344015	3.895563	-3.245248
	6	-1.995278	5.153364	-2.751593
	6	-1.678509	5.306904	-1.399797
	6	-1.720882	4.208030	-0.543725
	6	-0.882586	1.326684	0.343792
	6	-0.319142	-0.744599	1.501927
	6	0.986231	-0.271995	3.553424
	6	0.549379	-2.596185	2.822876
	6	-1.781340	0.914203	2.618278
	6	-1.694374	2.220909	3.113482
	6	-2.504137	2.615847	4.178930
	6	-3.382650	1.703930	4.767218
	6	-3.455409	0.398256	4.276723

	6	-2.667504	-0.001593	3.196756
	78	4.175128	0.189448	-0.178670
	17	4.616529	2.000569	-1.628543
	7	2.192325	0.549678	-0.341342
	6	1.491850	1.522330	0.140604
	6	2.109670	2.609486	0.974866
	17	3.729282	-1.591899	1.339973
	7	6.112481	-0.209552	-0.086660
	6	7.238705	-0.455522	-0.066636
	6	8.660578	-0.769335	-0.048177
	17	-1.028167	-0.527689	-2.573131
	17	-2.968307	-3.092236	0.973129
	1	-4.109208	-0.720318	0.105958
	1	0.261138	-2.252488	0.364924
	1	-5.415988	0.275932	-1.351652
	1	-6.309524	1.786196	-1.065904
	1	-6.235577	0.553172	0.212424
	1	-5.505822	2.862790	1.258739
	1	-4.874207	3.761312	-0.148195
	1	-3.776803	3.225154	1.148032
	1	-2.595678	1.796940	-2.783659
	1	-2.576183	3.766588	-4.298254
	1	-1.963258	6.010609	-3.417857
	1	-1.402313	6.282246	-1.009427
	1	-1.481825	4.321833	0.509757
	1	0.834162	0.766868	3.268156
	1	2.057457	-0.497452	3.516178
	1	0.608509	-0.421013	4.570691
	1	0.550813	-2.792175	3.898990
	1	1.523980	-2.876224	2.408703
	1	-0.247364	-3.181104	2.358320
	1	-0.987755	2.920081	2.674362
	1	-2.432052	3.630881	4.559228
	1	-4.003864	2.008150	5.604573
	1	-4.138952	-0.316411	4.726220
	1	-2.746820	-1.008227	2.795828
	1	1.666093	-0.084223	-0.946435
	1	3.059128	2.273719	1.394229
	1	1.426666	2.923711	1.770887
	1	2.307805	3.474015	0.331616
	1	9.243491	0.146385	0.090695
	1	8.950365	-1.234471	-0.995614
	1	8.879475	-1.461736	0.770450
$2_{(s)}$				
	78	-2.174200	-1.811685	-0.791531
	17	-1.043034	-3.794183	-1.449380
	17	-3.997468	-2.267389	-2.257984
	7	-3.286420	-0.183769	-0.134327
	7	-0.571234	-1.522771	0.492153

	7	−4.364864	1.872932	−0.144782
	7	−2.017664	1.815731	−0.245628
	7	0.262560	1.535153	−0.278716
	7	0.145635	−1.169122	2.687839
	7	−0.977058	0.543402	1.512146
	6	−3.239198	1.128301	−0.175550
	6	−5.658434	1.289092	−0.503890
	6	−4.435821	3.202028	0.468249
	6	−1.893867	2.938074	−1.162421
	6	−2.292716	2.799077	−2.492182
	6	−2.184475	3.890111	−3.356764
	6	−1.668160	5.103973	−2.901174
	6	−1.265547	5.231746	−1.569067
	6	−1.385875	4.153392	−0.694380
	6	−0.839803	1.284420	0.303271
	6	−0.453026	−0.758251	1.559037
	6	0.795635	−0.267036	3.642107
	6	0.368062	−2.597316	2.935578
	6	−1.768569	1.065438	2.599876
	6	−1.590285	2.392560	3.008205
	6	−2.349521	2.899751	4.063400
	6	−3.265719	2.081842	4.728378
	6	−3.427058	0.753985	4.326038
	6	−2.690592	0.242707	3.256421
	78	4.285570	0.103857	−0.188343
	17	4.712071	1.777209	−1.815890
	7	2.301303	0.453430	−0.363022
	6	1.554530	1.377647	0.151059
	6	2.099517	2.424529	1.078511
	17	3.859834	−1.566496	1.451532
	7	6.235465	−0.293162	−0.081038
	6	7.361345	−0.542442	−0.039777
	6	8.778102	−0.858454	0.006982
	17	−1.069453	−0.645248	−2.550305
	17	−3.287072	−3.009754	0.978095
	1	−4.196358	−0.543986	0.136566
	1	0.009848	−2.357584	0.491894
	1	−5.530450	0.512496	−1.260755
	1	−6.284354	2.082348	−0.921089
	1	−6.168366	0.866628	0.371955
	1	−5.266741	3.207238	1.181724
	1	−4.613274	3.970872	−0.290702
	1	−3.520035	3.426034	1.011102
	1	−2.663314	1.846470	−2.853545
	1	−2.491669	3.779999	−4.392714
	1	−1.576732	5.946450	−3.580733
	1	−0.865326	6.174110	−1.206094
	1	−1.087535	4.253906	0.344645
	1	0.849076	0.744387	3.245131
	1	1.814079	−0.625624	3.817031

	1	0.247540	−0.258746	4.590026
	1	0.361644	−2.759400	4.016420
	1	1.336772	−2.917104	2.534758
	1	−0.434087	−3.187161	2.487790
	1	−0.851785	3.019715	2.517020
	1	−2.208510	3.930817	4.374878
	1	−3.847119	2.475557	5.556990
	1	−4.137884	0.110336	4.836365
	1	−2.834095	−0.782985	2.931153
	1	1.812190	−0.160694	−1.016550
	1	3.074921	2.129104	1.468298
	1	1.401579	2.605951	1.902305
	1	2.212294	3.364577	0.525376
	1	9.360074	0.065138	0.085594
	1	9.065958	−1.389676	−0.905972
	1	8.986595	−1.492718	0.874357
3_(g)				
	78	1.561663	−1.171304	−1.808231
	17	−0.377641	−2.212254	−2.620481
	17	2.867372	−3.132510	−1.846289
	7	3.247873	−0.247420	−1.072996
	7	0.437758	0.539303	−1.825869
	7	4.901109	−0.043130	0.575274
	7	2.623763	−0.007212	1.181863
	7	0.325282	−0.161778	1.343576
	7	−0.117066	2.792316	−1.458107
	7	1.271454	1.633482	0.068976
	6	3.605543	−0.085569	0.169919
	6	5.945407	−0.624175	−0.263407
	6	5.349342	0.691342	1.754155
	6	2.730581	−0.967818	2.270514
	6	2.836600	−2.329772	1.980695
	6	2.938120	−3.239604	3.033917
	6	2.917829	−2.795583	4.357455
	6	2.799117	−1.431898	4.634750
	6	2.710564	−0.512632	3.589660
	6	1.330014	0.449623	0.860404
	6	0.484914	1.623778	−1.107958
	6	−0.715073	3.698663	−0.473921
	6	−0.637218	2.937342	−2.817725
	6	2.206622	2.697873	0.304119
	6	2.360189	3.208308	1.599196
	6	3.263539	4.243952	1.838530
	6	4.000528	4.791646	0.786456
	6	3.835448	4.289748	−0.506201
	6	2.950398	3.239610	−0.750354
	78	−3.843790	−0.092653	0.412146
	17	−4.021776	−1.640415	2.185830
	7	−1.829965	−0.273795	0.480788

	6	-0.997842	0.218272	1.336498
	6	-1.451148	1.083107	2.479808
	17	-3.668301	1.542394	-1.317732
	7	-5.818569	0.004626	0.303073
	6	-6.968989	0.021247	0.227466
	6	-8.421866	0.033572	0.129175
	1	4.012688	-0.191066	-1.737901
	1	-0.330586	0.494326	-2.492325
	1	5.542003	-1.469487	-0.827386
	1	6.745593	-0.992664	0.385455
	1	6.378716	0.110648	-0.957618
	1	6.164508	1.366715	1.467821
	1	5.709994	0.006965	2.530637
	1	4.533518	1.290584	2.154077
	1	2.817429	-2.673596	0.948843
	1	3.014629	-4.300242	2.813450
	1	2.987325	-3.510646	5.172334
	1	2.778512	-1.082057	5.663081
	1	2.619798	0.550655	3.793661
	1	-0.319020	3.496715	0.519357
	1	-1.802356	3.558950	-0.461636
	1	-0.477606	4.733804	-0.741348
	1	-0.719777	4.005658	-3.037754
	1	-1.628003	2.478169	-2.921568
	1	0.058402	2.485054	-3.529989
	1	1.766504	2.799238	2.411962
	1	3.375711	4.634099	2.846206
	1	4.693615	5.606972	0.971706
	1	4.404290	4.709740	-1.330972
	1	2.832256	2.840300	-1.752288
	1	-1.417286	-0.893350	-0.223936
	1	-2.472548	1.428398	2.314571
	1	-0.774912	1.935540	2.606810
	1	-1.426903	0.489975	3.400600
	1	-8.863187	0.120654	1.126836
	1	-8.770500	-0.895281	-0.333109
	1	-8.748143	0.880304	-0.482444
3_(s)				
	78	1.930837	-2.109528	-0.547603
	17	0.277575	-3.789444	-0.792178
	17	3.356000	-3.559294	0.678026
	7	3.410491	-0.693102	-0.402328
	7	0.693947	-0.937086	-1.679869
	7	4.768133	0.852116	0.725144
	7	2.432393	0.889848	1.036323
	7	0.132387	0.759801	1.029288
	7	0.066296	0.869359	-3.030664
	7	1.264668	1.240424	-1.025210
	6	3.566133	0.322783	0.404985

	6	5.997925	0.139128	0.386314
	6	4.951693	2.241246	1.147209
	6	2.417519	0.913208	2.489935
	6	2.683567	−0.260824	3.197952
	6	2.677389	−0.233768	4.593496
	6	2.392535	0.951073	5.274702
	6	2.117387	2.118024	4.557194
	6	2.136042	2.104746	3.162726
	6	1.208086	0.942105	0.365265
	6	0.643174	0.347580	−1.924614
	6	−0.529323	2.205747	−3.083126
	6	−0.273932	−0.004800	−4.152492
	6	2.143956	2.275802	−1.508973
	6	2.105569	3.541527	−0.911447
	6	2.947361	4.553960	−1.372894
	6	3.811947	4.317379	−2.443989
	6	3.835656	3.057830	−3.047160
	6	3.012907	2.032215	−2.579051
	78	−4.028707	0.122204	0.319277
	17	−4.262720	0.360645	2.669911
	7	−2.018347	0.085463	0.533565
	6	−1.165496	1.047268	0.691083
	6	−1.587158	2.488324	0.700617
	17	−3.800894	−0.105675	−2.038374
	7	−6.012696	0.083723	0.131265
	6	−7.161668	0.041216	0.033096
	6	−8.608120	−0.015963	−0.085490
	1	4.252278	−0.955562	−0.906922
	1	0.031128	−1.494110	−2.213455
	1	5.873517	−0.935751	0.537109
	1	6.790592	0.489957	1.051349
	1	6.305235	0.329814	−0.651161
	1	5.619415	2.744496	0.438356
	1	5.399838	2.278766	2.145557
	1	4.001588	2.768786	1.156225
	1	2.876183	−1.187362	2.665028
	1	2.882386	−1.147079	5.144666
	1	2.381396	0.965562	6.360958
	1	1.895011	3.043009	5.081827
	1	1.932803	3.012566	2.602918
	1	−0.430262	2.709625	−2.124325
	1	−1.595345	2.113654	−3.316750
	1	−0.043345	2.807537	−3.858718
	1	−0.310683	0.602612	−5.060673
	1	−1.251460	−0.482857	−4.010236
	1	0.490485	−0.775985	−4.278903
	1	1.411387	3.734975	−0.098560
	1	2.912305	5.533028	−0.903574
	1	4.457906	5.110277	−2.809768
	1	4.503127	2.863884	−3.882105

	1	3.046187	1.053089	-3.045141
	1	-1.605664	-0.847672	0.585979
	1	-2.606602	2.596984	0.326770
	1	-0.902493	3.093338	0.097416
	1	-1.546075	2.864726	1.729498
	1	-9.052735	0.866766	0.384913
	1	-8.981836	-0.916043	0.413215
	1	-8.891505	-0.044344	-1.142286
$4_{(g)}$				
	78	1.752012	-0.747998	0.084752
	17	3.830727	-1.082312	-0.973996
	17	2.178604	-2.390870	1.729779
	7	-0.004640	-0.398151	1.144493
	7	1.479798	0.743381	-1.335354
	7	-2.107940	-0.823826	2.022049
	7	-1.908132	-0.351318	-0.270088
	7	-1.584104	0.191311	-2.502039
	7	1.086456	3.025743	-1.646065
	7	-0.620904	1.612913	-0.826445
	6	-1.295230	-0.522602	0.972238
	6	-1.580998	-1.536752	3.184610
	6	-3.462178	-0.295182	2.162903
	6	-2.950797	-1.285421	-0.660784
	6	-2.710154	-2.657859	-0.593501
	6	-3.727268	-3.548872	-0.940139
	6	-4.967849	-3.074394	-1.367211
	6	-5.194557	-1.698168	-1.445906
	6	-4.189900	-0.802077	-1.086953
	6	-1.351374	0.461195	-1.284891
	6	0.687390	1.782120	-1.279001
	6	0.185757	4.025515	-2.213161
	6	2.509328	3.369071	-1.649808
	6	-1.231591	2.527209	0.096147
	6	-2.561343	2.921385	-0.101657
	6	-3.166555	3.798618	0.798787
	6	-2.443887	4.303105	1.881842
	6	-1.114819	3.915430	2.066561
	6	-0.505654	3.019209	1.187317
	17	2.698110	0.967045	1.505297
	17	0.767958	-2.381667	-1.321443
	1	0.269144	-0.326467	2.119656
	1	2.337257	0.854001	-1.870922
	1	-1.198259	0.911805	-3.112526
	1	-0.713238	-2.135351	2.898907
	1	-2.361131	-2.205369	3.562767
	1	-1.296151	-0.848655	3.993203
	1	-3.559372	0.163390	3.154137
	1	-4.210487	-1.089363	2.062407
	1	-3.649057	0.470479	1.411967

	1	-1.728074	-3.017987	-0.306104
	1	-3.537276	-4.617194	-0.891354
	1	-5.753093	-3.772058	-1.644439
	1	-6.155735	-1.320250	-1.782992
	1	-4.363132	0.268235	-1.144304
	1	-0.808334	3.604724	-2.356747
	1	0.573217	4.351230	-3.185916
	1	0.107707	4.897593	-1.553839
	1	2.608896	4.428294	-1.393326
	1	2.966022	3.207739	-2.635660
	1	3.033852	2.775767	-0.897603
	1	-3.110814	2.551287	-0.963106
	1	-4.198648	4.099341	0.641519
	1	-2.913386	4.993342	2.576713
	1	-0.547449	4.297163	2.910709
	1	0.515123	2.685270	1.352149
4_(s)				
	78	1.812114	-0.640740	0.087520
	17	3.928916	-0.809465	-0.990847
	17	2.354521	-2.399495	1.605500
	7	0.050534	-0.440955	1.161793
	7	1.459799	0.908298	-1.235529
	7	-2.029809	-0.973572	2.038558
	7	-1.855382	-0.494245	-0.252962
	7	-1.546318	0.115220	-2.471669
	7	0.814590	3.109261	-1.672957
	7	-0.726288	1.572157	-0.756887
	6	-1.239308	-0.636452	0.991982
	6	-1.461271	-1.569071	3.248167
	6	-3.411639	-0.508258	2.177536
	6	-2.865296	-1.458002	-0.656780
	6	-2.588475	-2.824617	-0.598881
	6	-3.573588	-3.742682	-0.969403
	6	-4.820422	-3.300101	-1.412648
	6	-5.085184	-1.929455	-1.480490
	6	-4.113410	-1.007361	-1.096709
	6	-1.360007	0.382915	-1.243985
	6	0.553984	1.861546	-1.232847
	6	-0.207936	3.985044	-2.249979
	6	2.191921	3.582207	-1.823135
	6	-1.414246	2.448645	0.150816
	6	-2.776308	2.716663	-0.036896
	6	-3.445590	3.560221	0.850941
	6	-2.759103	4.156923	1.910674
	6	-1.398488	3.894419	2.086732
	6	-0.724678	3.032837	1.220185
	17	2.699425	0.974778	1.640828
	17	0.939192	-2.239845	-1.443299
	1	0.315308	-0.344161	2.137081

	1	2.295608	1.091993	-1.783990
	1	-1.239247	0.890804	-3.060171
	1	-0.586792	-2.174700	3.003302
	1	-2.219712	-2.217099	3.695965
	1	-1.180763	-0.803454	3.984159
	1	-3.508982	0.004775	3.141031
	1	-4.110934	-1.350444	2.151662
	1	-3.660723	0.197392	1.388163
	1	-1.607455	-3.167519	-0.289795
	1	-3.353621	-4.805583	-0.924056
	1	-5.581221	-4.017062	-1.708403
	1	-6.052608	-1.575473	-1.825911
	1	-4.320308	0.057566	-1.141499
	1	-1.156390	3.460099	-2.348899
	1	0.120843	4.301139	-3.245978
	1	-0.349423	4.872964	-1.624932
	1	2.200767	4.664479	-1.669283
	1	2.581989	3.368089	-2.826461
	1	2.837823	3.118373	-1.075376
	1	-3.305663	2.279086	-0.878198
	1	-4.502376	3.762383	0.700490
	1	-3.280203	4.821482	2.593816
	1	-0.856236	4.348947	2.911114
	1	0.324856	2.806446	1.378447
5 _(g)				
	78	-2.161644	-1.947719	-0.548344
	17	-0.854896	-3.851847	-0.959520
	17	-3.961182	-2.765961	-1.846707
	7	-3.463557	-0.366600	-0.114916
	7	-0.562255	-1.310190	0.628110
	7	-4.771342	1.527463	-0.439812
	7	-2.428903	1.738359	-0.433236
	7	-0.132329	1.702671	-0.443215
	7	0.054295	-0.659370	2.789170
	7	-1.271066	0.762544	1.436686
	6	-3.563140	0.917601	-0.316785
	6	-5.945633	0.755432	-0.844922
	6	-5.038514	2.882550	0.038762
	6	-2.397046	2.730405	-1.497198
	6	-2.646940	2.343619	-2.813924
	6	-2.627834	3.308923	-3.821798
	6	-2.345101	4.641805	-3.519820
	6	-2.083644	5.016300	-2.199719
	6	-2.116599	4.062325	-1.184127
	6	-1.207279	1.387386	0.161366
	6	-0.566631	-0.448447	1.615167
	6	0.571299	0.404727	3.651866
	6	0.469351	-2.018757	3.158567
	6	-2.179092	1.254034	2.441717

	6	-2.198013	2.621866	2.741724
	6	-3.070017	3.107007	3.716663
	6	-3.904675	2.228539	4.410720
	6	-3.870593	0.863965	4.116094
	6	-3.019917	0.369977	3.125944
	78	3.869832	0.216483	-0.150585
	17	3.823373	-0.401880	-2.443178
	7	1.909036	0.670112	-0.350533
	6	1.160251	1.669264	0.003016
	6	1.641832	2.888640	0.732362
	17	3.982867	0.787103	2.191186
	7	5.802913	-0.358092	-0.046514
	6	6.897832	-0.705366	-0.025821
	6	8.283270	-1.148190	-0.004772
	17	-1.223354	-0.897306	-2.461753
	17	-3.089434	-2.960192	1.433051
	17	3.174727	-1.996556	0.453516
	17	4.601565	2.401494	-0.777421
	1	-4.340546	-0.805508	0.150116
	1	0.145022	-2.041973	0.678371
	1	-5.644251	-0.094613	-1.461132
	1	-6.597171	1.405870	-1.436562
	1	-6.516015	0.391843	0.021441
	1	-5.906150	2.855278	0.708374
	1	-5.252585	3.559780	-0.795354
	1	-4.187296	3.261158	0.601319
	1	-2.814080	1.297112	-3.046074
	1	-2.815781	3.008857	-4.848414
	1	-2.321339	5.386259	-4.310381
	1	-1.859146	6.051266	-1.958154
	1	-1.922479	4.348105	-0.154256
	1	0.340280	1.382652	3.236638
	1	1.658638	0.307552	3.724744
	1	0.120909	0.325273	4.647246
	1	0.480506	-2.081618	4.250029
	1	1.471856	-2.238792	2.774926
	1	-0.251720	-2.741348	2.770139
	1	-1.523949	3.300142	2.225297
	1	-3.079916	4.168815	3.945903
	1	-4.573845	2.605279	5.178739
	1	-4.518952	0.173910	4.648439
	1	-3.018160	-0.686829	2.873391
	1	1.426072	-0.039440	-0.908056
	1	2.610286	2.731321	1.200500
	1	0.899637	3.177273	1.484114
	1	1.723400	3.707921	0.009930
	1	8.924205	-0.370329	-0.430491
	1	8.383394	-2.063060	-0.596624
	1	8.591672	-1.348228	1.025687

5 _(s)				
	78	-2.531482	-1.875334	-0.537313
	17	-1.465456	-3.963530	-0.893648
	17	-4.347476	-2.489751	-1.951656
	7	-3.592497	-0.129661	-0.155590
	7	-0.933243	-1.450123	0.719710
	7	-4.580297	1.937135	-0.546962
	7	-2.233082	1.773792	-0.530192
	7	0.032888	1.444585	-0.403219
	7	-0.274927	-0.823998	2.873662
	7	-1.314804	0.741255	1.439613
	6	-3.489222	1.155228	-0.403056
	6	-5.882129	1.344207	-0.862717
	6	-4.631228	3.340664	-0.125478
	6	-2.022396	2.757671	-1.582729
	6	-2.314456	2.440019	-2.909223
	6	-2.117864	3.403523	-3.900838
	6	-1.618650	4.664720	-3.572969
	6	-1.318391	4.969217	-2.242519
	6	-1.525926	4.019631	-1.243679
	6	-1.107019	1.305451	0.151754
	6	-0.825949	-0.555163	1.680469
	6	0.346772	0.185201	3.734951
	6	-0.098175	-2.211062	3.316879
	6	-2.144523	1.421819	2.404111
	6	-1.977949	2.797636	2.602223
	6	-2.769161	3.462078	3.539914
	6	-3.707451	2.755267	4.295077
	6	-3.860057	1.380684	4.099731
	6	-3.090914	0.709051	3.148429
	78	4.068646	0.048079	-0.121564
	17	4.021557	-0.443895	-2.457353
	7	2.087458	0.453904	-0.281891
	6	1.298070	1.419015	0.096611
	6	1.723595	2.598536	0.918334
	17	4.179635	0.493070	2.236600
	7	6.022693	-0.477909	-0.060190
	6	7.126187	-0.803773	-0.055283
	6	8.515317	-1.219651	-0.053671
	17	-1.369951	-1.003946	-2.420072
	17	-3.700947	-2.765952	1.373660
	17	3.459609	-2.216762	0.361461
	17	4.738376	2.287266	-0.636264
	1	-4.526839	-0.409249	0.128157
	1	-0.368967	-2.287448	0.844181
	1	-5.755995	0.463997	-1.495780
	1	-6.468175	2.087278	-1.409756
	1	-6.432696	1.068182	0.046271
	1	-5.457708	3.458516	0.584109
	1	-4.804937	3.993986	-0.985960

	1	-3.710203	3.628834	0.375397
	1	-2.666877	1.448578	-3.169362
	1	-2.343203	3.155430	-4.933924
	1	-1.460775	5.407086	-4.350075
	1	-0.929888	5.948679	-1.978517
	1	-1.307444	4.256569	-0.206669
	1	0.410555	1.142847	3.223950
	1	1.359960	-0.145479	3.981638
	1	-0.229419	0.300678	4.658895
	1	-0.145753	-2.226069	4.408499
	1	0.874765	-2.605499	3.001333
	1	-0.898390	-2.839121	2.921461
	1	-1.227179	3.341796	2.036931
	1	-2.636292	4.529587	3.690311
	1	-4.313654	3.271700	5.033573
	1	-4.590126	0.824155	4.680416
	1	-3.229166	-0.354370	2.980755
	1	1.629282	-0.242080	-0.873029
	1	2.714806	2.469039	1.343987
	1	0.995331	2.760945	1.720020
	1	1.718123	3.488232	0.279192
	1	9.127690	-0.446983	-0.528922
	1	8.612610	-2.156859	-0.610780
	1	8.850643	-1.370198	0.977226
2' (g)				
	78	-3.191305	-1.852371	-0.050371
	17	-2.713689	-3.903882	0.977577
	17	-3.553788	-2.794422	-2.176974
	7	-3.706505	-0.080450	-0.958855
	7	-2.864359	-1.064635	1.812330
	7	-3.402765	1.670638	-2.482512
	7	-1.652008	1.066813	-1.010364
	7	-0.199231	0.496665	0.821523
	7	-2.655499	0.528292	3.534712
	7	-2.347365	1.139370	1.265975
	6	-2.983797	0.874223	-1.465094
	6	-4.512966	1.239942	-3.327931
	6	-2.941658	3.041673	-2.679628
	6	-0.614269	1.079111	-2.028452
	6	-0.599419	0.069684	-2.996156
	6	0.375337	0.102793	-3.993145
	6	1.332518	1.118901	-4.011854
	6	1.313789	2.116219	-3.035634
	6	0.330073	2.107449	-2.047814
	6	-1.329713	0.844147	0.330365
	6	-2.613923	0.140837	2.228336
	6	-1.738733	1.539187	4.065957
	6	-3.232545	-0.373330	4.525432
	6	-3.091424	2.358348	1.236312

	6	-2.434756	3.573067	0.999530
	6	-3.162609	4.763023	0.973458
	6	-4.538534	4.752864	1.209944
	6	-5.186536	3.541902	1.464943
	6	-4.472535	2.344300	1.468166
	78	3.992917	0.018453	0.273039
	17	4.241919	1.032406	2.429471
	7	2.032649	0.463635	0.449893
	6	0.896262	-0.156569	0.316187
	6	0.750858	-1.569442	-0.154315
	17	3.799838	-0.968808	-1.895439
	7	5.984223	-0.306824	0.175720
	6	7.114898	-0.505131	0.130682
	6	8.546351	-0.758358	0.074152
	17	3.763243	-2.111881	1.319838
	17	4.280612	2.180128	-0.733026
	1	-4.669068	-0.083328	-1.281368
	1	-2.829943	-1.799739	2.516967
	1	-4.502852	0.151511	-3.431706
	1	-4.383984	1.684143	-4.319131
	1	-5.486549	1.563413	-2.931622
	1	-3.802217	3.721348	-2.654471
	1	-2.433548	3.142690	-3.645058
	1	-2.258316	3.328968	-1.884178
	1	-1.330064	-0.735072	-2.960696
	1	0.396888	-0.683772	-4.741435
	1	2.105423	1.123933	-4.774044
	1	2.074106	2.889502	-3.026917
	1	0.308924	2.883565	-1.287748
	1	-1.255949	2.075322	3.251739
	1	-0.958578	1.060584	4.671819
	1	-2.289115	2.249906	4.691288
	1	-3.521948	0.213441	5.401731
	1	-2.522356	-1.148440	4.848338
	1	-4.124913	-0.855502	4.117487
	1	-1.358156	3.584992	0.853952
	1	-2.646174	5.700897	0.789578
	1	-5.100578	5.682048	1.202504
	1	-6.256600	3.524897	1.651622
	1	-4.977728	1.400260	1.646999
	1	1.949219	1.391830	0.860255
	1	1.521702	-1.812072	-0.885923
	1	-0.249468	-1.738943	-0.558071
	1	0.879336	-2.235763	0.705750
	1	8.795895	-1.600443	0.726659
	1	9.091314	0.130344	0.406202
	1	8.837312	-0.998693	-0.952812
$2'_{(s)}$				
	78	3.089786	-1.888249	0.465533

	17	2.614135	−4.133538	−0.125386
	17	3.636417	−2.492718	2.695293
	7	3.638106	0.017842	1.005183
	7	2.649077	−1.479146	−1.493560
	7	3.505334	2.093183	2.076375
	7	1.684541	1.319838	0.775591
	7	0.168504	0.454068	−0.865346
	7	2.568402	−0.299680	−3.523064
	7	2.351383	0.830233	−1.453653
	6	3.000047	1.123962	1.278949
	6	4.642649	1.798227	2.947127
	6	3.213118	3.517974	1.908312
	6	0.656217	1.796180	1.684797
	6	0.457076	1.148064	2.906031
	6	−0.504814	1.637460	3.790855
	6	−1.269392	2.755721	3.453092
	6	−1.069450	3.391709	2.225728
	6	−0.101971	2.919173	1.339900
	6	1.337723	0.829142	−0.480294
	6	2.512572	−0.372628	−2.176011
	6	1.863063	0.729772	−4.290152
	6	3.046921	−1.441165	−4.300067
	6	3.207723	1.955667	−1.696646
	6	2.676543	3.251629	−1.696093
	6	3.508824	4.342040	−1.951528
	6	4.862167	4.146278	−2.233901
	6	5.383518	2.850439	−2.249552
	6	4.566272	1.754416	−1.972104
	78	−4.014041	−0.041533	−0.249608
	17	−4.247761	0.383370	−2.600525
	7	−2.064524	0.461805	−0.476519
	6	−0.905259	−0.083547	−0.220125
	6	−0.723806	−1.340744	0.569720
	17	−3.846875	−0.444572	2.100251
	7	−5.996561	−0.446491	−0.118059
	6	−7.118965	−0.689884	−0.047687
	6	−8.533151	−0.997867	0.042134
	17	−3.658721	−2.355253	−0.731733
	17	−4.460519	2.274345	0.182734
	1	4.608747	0.034895	1.304920
	1	2.552513	−2.333433	−2.037978
	1	4.554352	0.789996	3.358685
	1	4.631715	2.512748	3.774137
	1	5.600436	1.896145	2.417591
	1	4.143057	4.046063	1.666503
	1	2.799082	3.931722	2.833383
	1	2.512287	3.677852	1.093863
	1	1.039832	0.268444	3.161141
	1	−0.662198	1.132043	4.739089
	1	−2.022683	3.128114	4.141054

	1	−1.662790	4.260578	1.957047
	1	0.067406	3.421602	0.392062
	1	1.321753	1.400215	−3.625830
	1	1.138482	0.246182	−4.954826
	1	2.570677	1.307193	−4.894394
	1	3.396348	−1.075115	−5.268639
	1	2.250674	−2.177959	−4.471796
	1	3.882826	−1.926746	−3.789817
	1	1.617941	3.407090	−1.511078
	1	3.089325	5.344041	−1.948585
	1	5.504007	4.996237	−2.446471
	1	6.434676	2.686983	−2.469617
	1	4.980456	0.751242	−1.972667
	1	−1.997035	1.290553	−1.065513
	1	−1.561853	−1.513297	1.242523
	1	0.214282	−1.300925	1.128721
	1	−0.647292	−2.184627	−0.124292
	1	−8.732729	−1.943691	−0.471450
	1	−9.111287	−0.196836	−0.428900
	1	−8.820151	−1.085789	1.094680
[Pt^{IV}R]_(g)				
	78	0.000003	0.000216	0.000102
	17	0.001041	−2.299496	−0.663901
	7	−1.975192	−0.000265	−0.000907
	6	−3.123028	−0.000880	−0.001259
	6	−4.576879	−0.001638	−0.001690
	17	−0.001071	2.299840	0.663932
	7	1.975201	0.000204	0.001002
	6	3.123038	−0.000294	0.000795
	6	4.576830	−0.000995	0.000450
	17	0.001696	0.664203	−2.299509
	17	−0.001658	−0.663633	2.299827
	1	−4.942646	−0.739054	−0.722563
	1	−4.943747	0.990971	−0.279807
	1	−4.943368	−0.257465	0.997031
	1	4.942596	−1.006682	−0.227699
	1	4.943666	0.304073	0.985101
	1	4.943286	0.699024	−0.756432
[Pt^{IV}R]_(s)				
	78	−0.000004	0.003291	0.000420
	17	−0.000434	−2.287211	0.698801
	7	1.981747	0.001493	0.002826
	6	3.131515	−0.007142	0.002327
	6	4.579987	−0.020899	−0.001897
	17	0.000422	2.293390	−0.697789
	7	−1.981766	0.000577	−0.002793
	6	−3.131532	−0.007494	−0.003657
	6	−4.580016	−0.021341	−0.003723

	17	-0.003075	0.701629	2.290656
	17	0.003157	-0.694921	-2.289934
	1	4.937510	-0.765966	0.716032
	1	4.953070	0.968959	0.279076
	1	4.936541	-0.276546	-1.004822
	1	-4.932480	-1.029041	0.238726
	1	-4.945581	0.266563	-0.994358
	1	-4.949538	0.687016	0.744575
[Pt^{II}R]_(g)				
	78	-0.000003	-0.000019	0.000512
	17	-0.001718	2.368921	0.000179
	7	-1.962823	-0.001175	0.000348
	6	-3.114779	-0.001257	-0.000516
	6	-4.570259	-0.000486	-0.002408
	17	0.001718	-2.368945	0.000179
	7	1.962827	0.001009	0.000378
	6	3.114772	0.001099	-0.000532
	6	4.570294	0.000838	-0.002431
	1	-4.940027	1.001081	-0.242468
	1	-4.943916	-0.293385	0.983683
	1	-4.941279	-0.709283	-0.749154
	1	4.940915	0.712768	-0.746361
	1	4.940679	-0.999566	-0.246236
	1	4.943668	0.290260	0.984786
[Pt^{II}R]_(s)				
	78	-0.000001	-0.000043	0.004354
	17	0.002335	2.373044	0.004476
	7	-1.971395	0.001892	0.001112
	6	-3.124309	0.002160	-0.007308
	6	-4.575455	0.001064	-0.022064
	17	-0.002330	-2.373129	0.004473
	7	1.971393	-0.001977	0.001037
	6	3.124307	-0.002038	-0.007376
	6	4.575455	-0.000587	-0.022020
	1	-4.940445	0.992491	-0.308249
	1	-4.953230	-0.250641	0.974037
	1	-4.934824	-0.740112	-0.742997
	1	4.934676	0.738794	-0.744867
	1	4.940761	-0.992660	-0.305532
	1	4.953065	0.253891	0.973443

Figure S1. IR spectrum of **2a**.

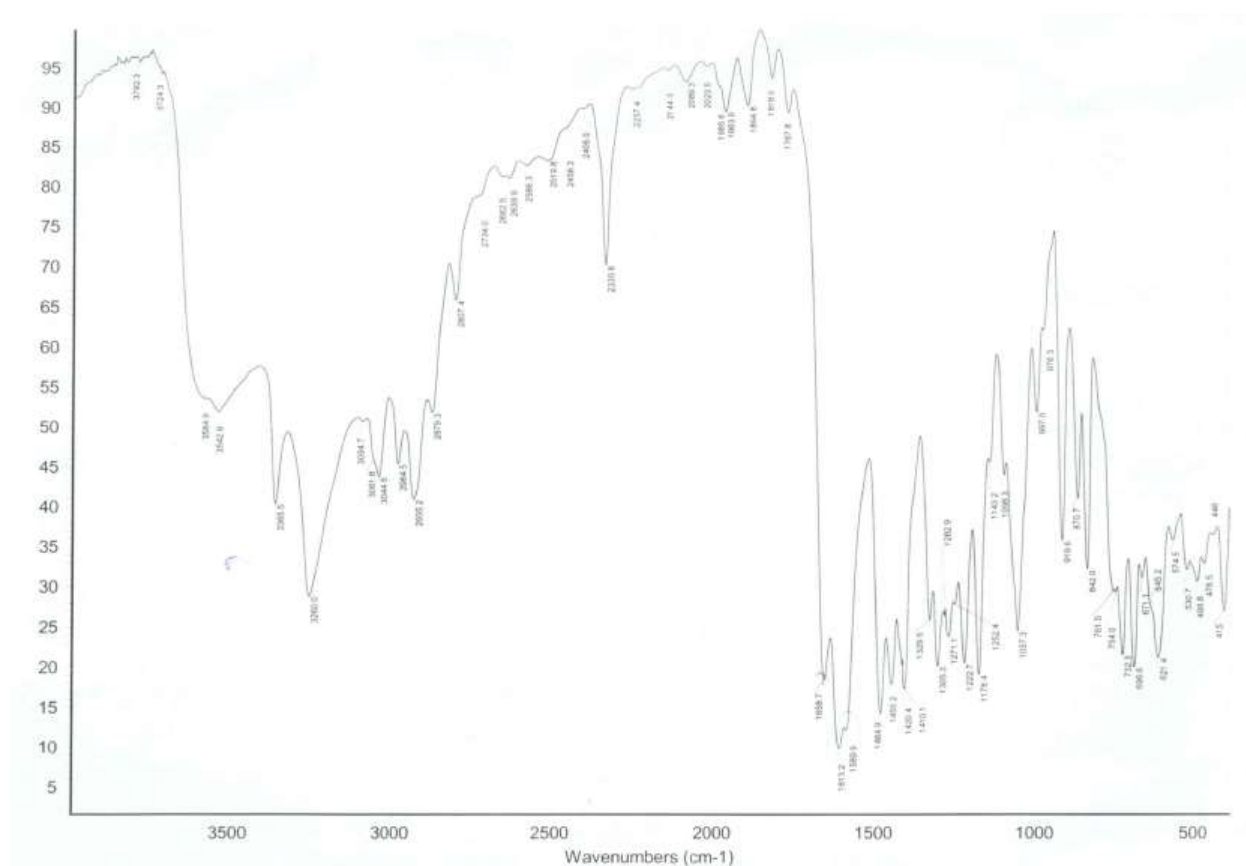


Figure S2. IR spectrum of **2a**·2CDCl₃.

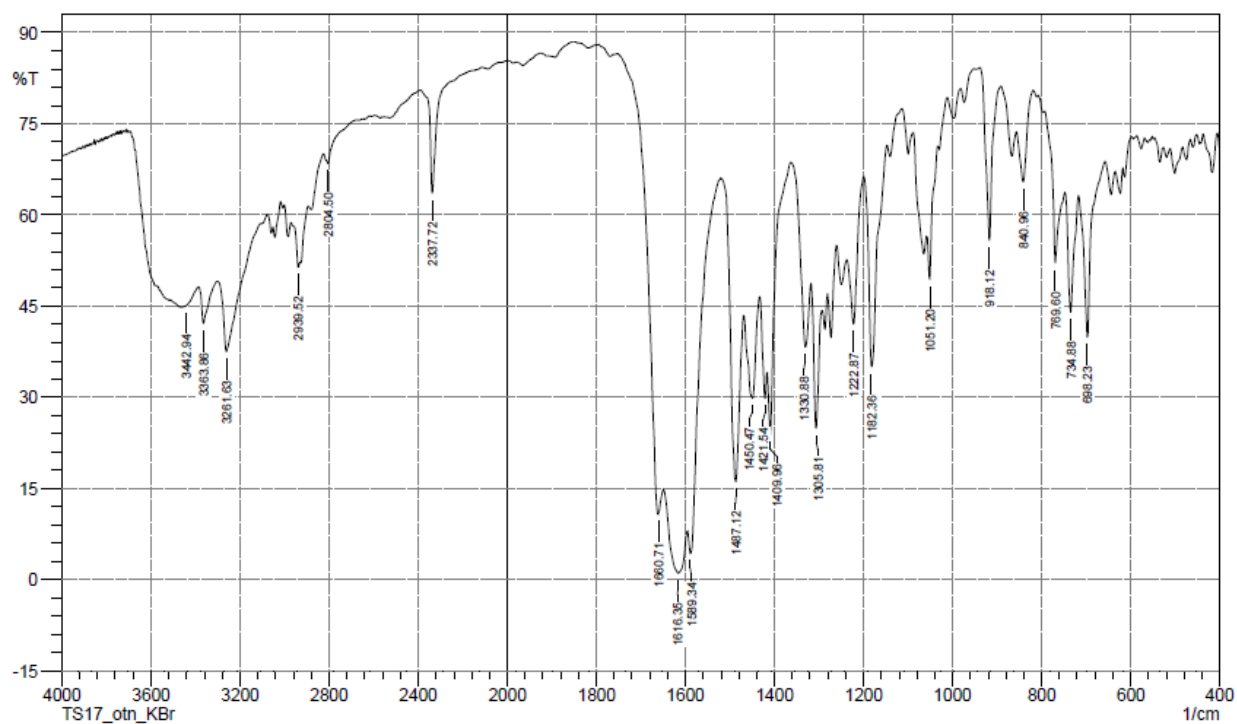


Figure S3. IR spectrum of **2b**

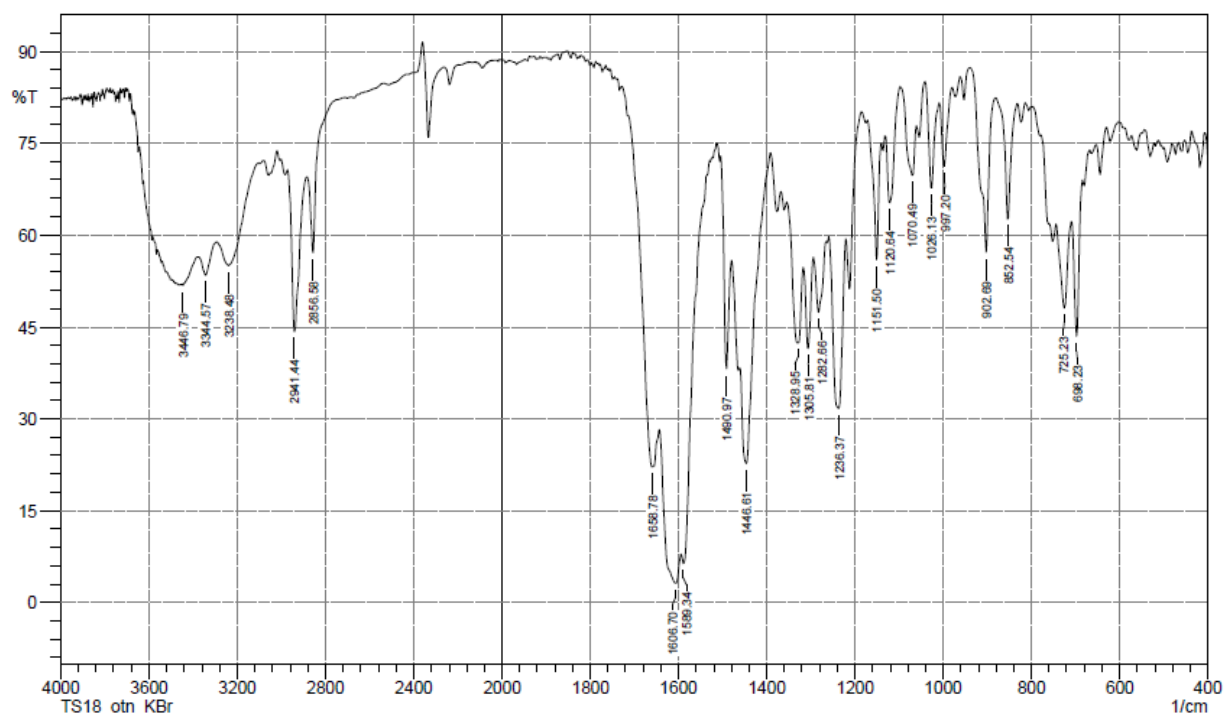


Figure S4. IR spectrum of **3a**

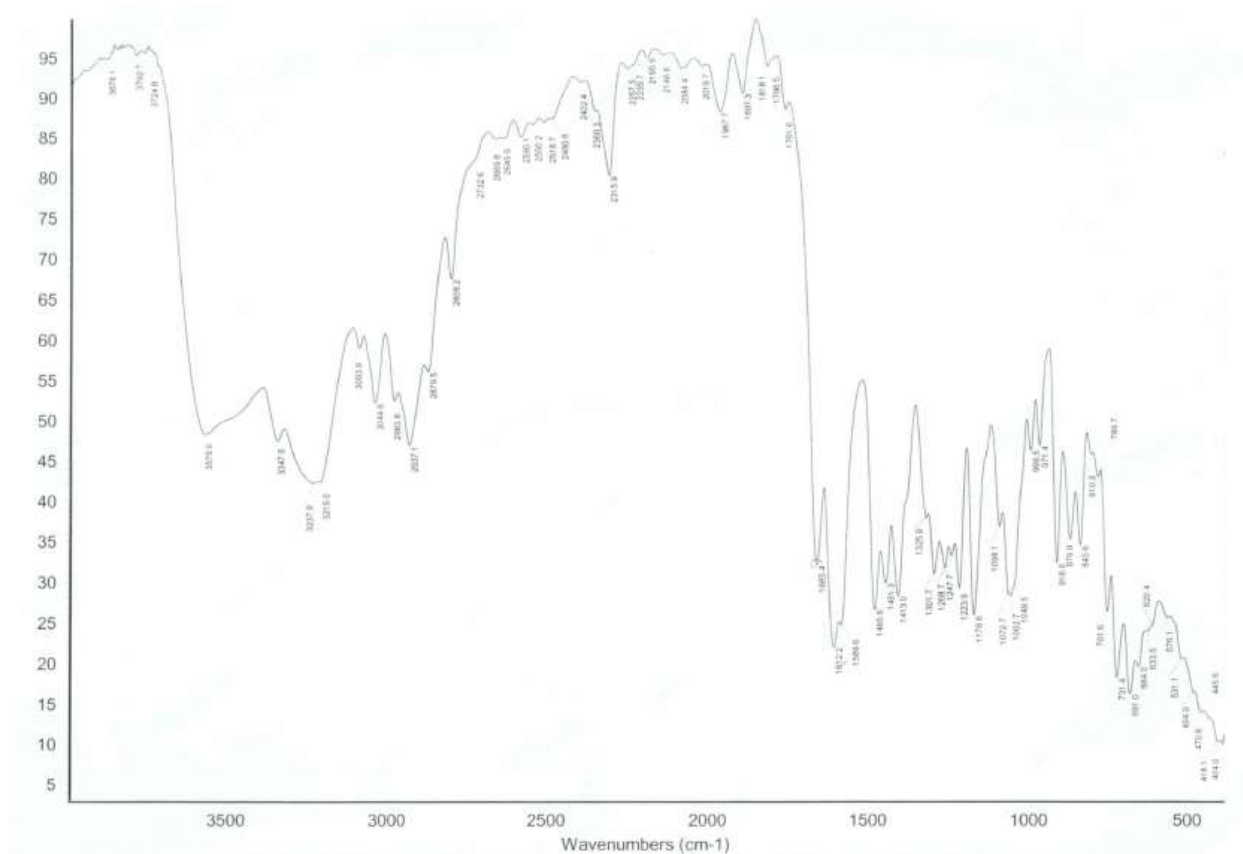


Figure S5. IR spectra of **3b**.

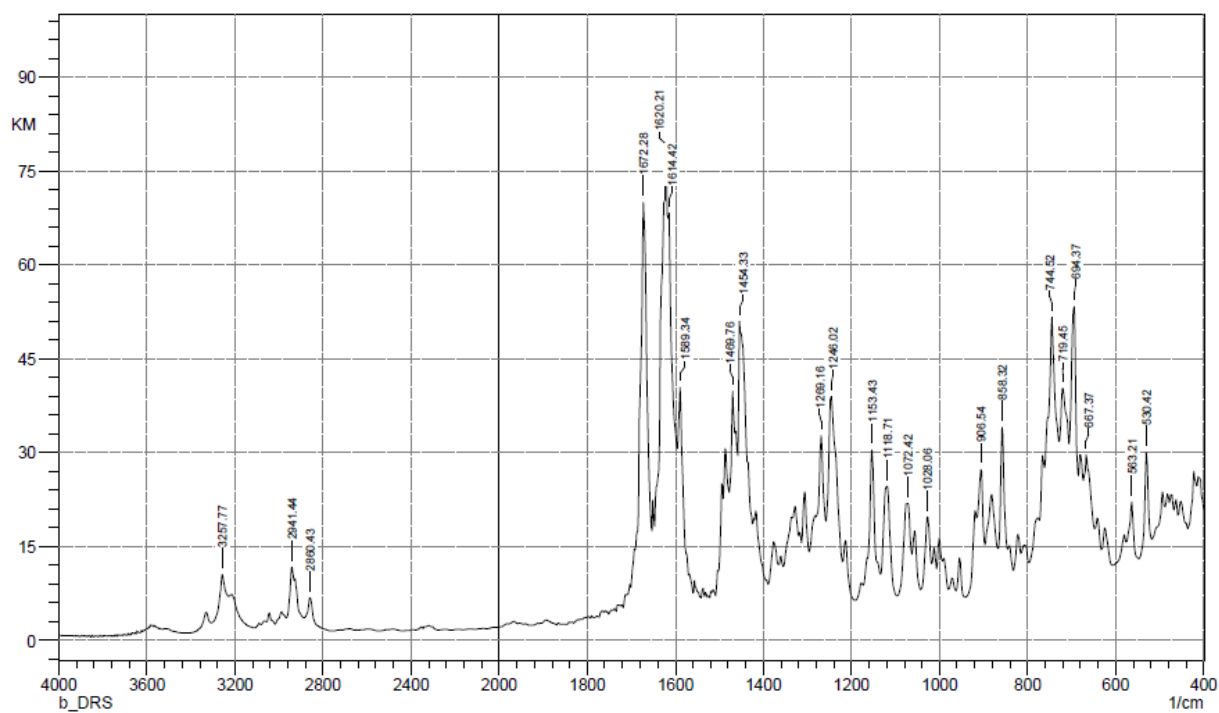
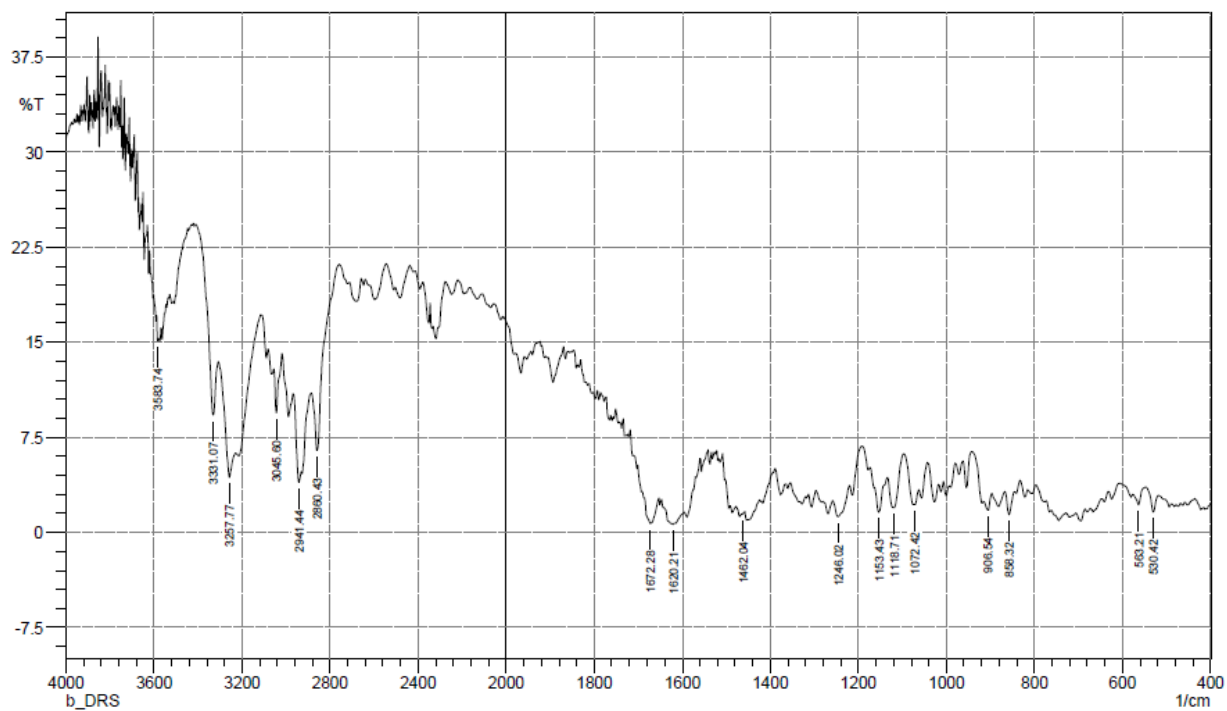


Figure S6. IR spectrum of **6a**.

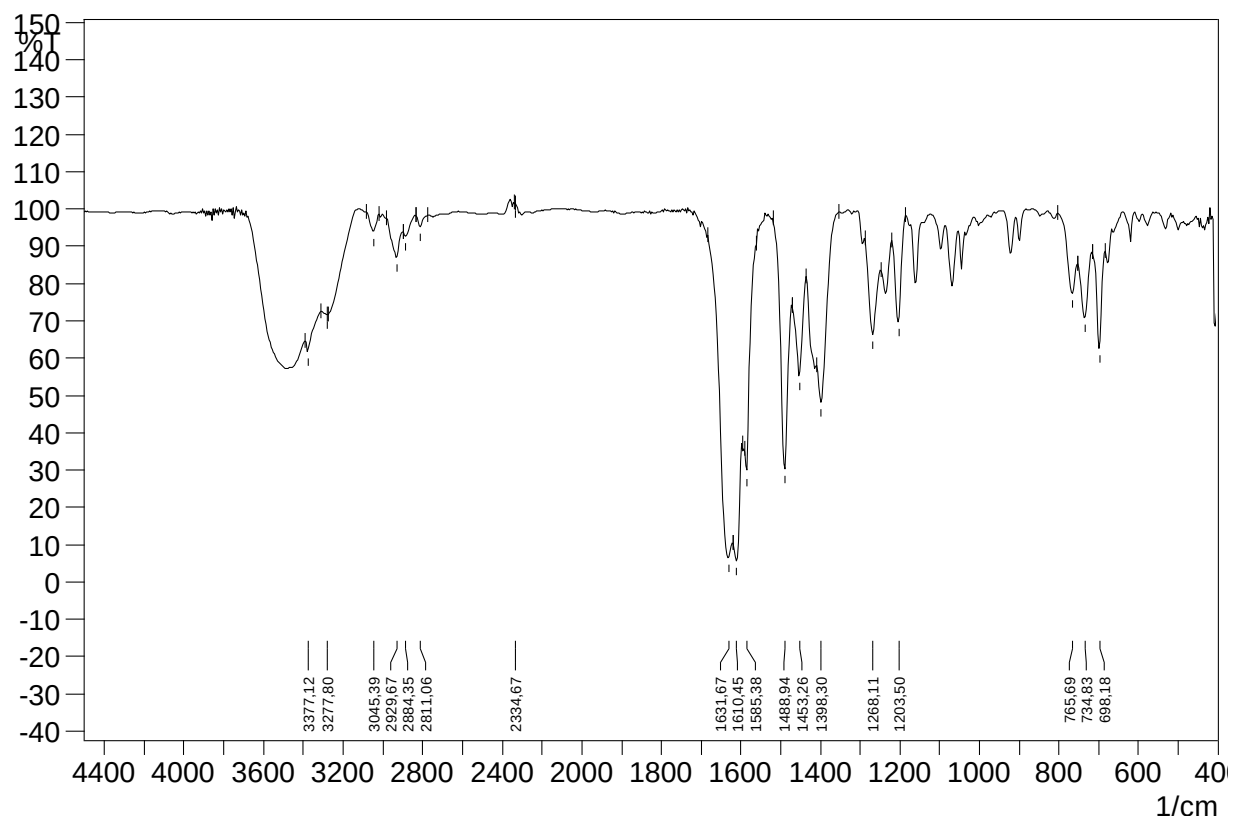


Figure S7. IR spectrum of **6b**.

